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# The time-dependent quantum harmonic oscillator revisited: Applications to quantum field theory

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## A B S T R A C T

In this article, we formulate the study of the unitary time evolution of systems consisting of an infinite number of uncoupled time-dependent harmonic oscillators in mathematically rigorous terms. We base this analysis on the theory of a single one-dimensional time-dependent oscillator, for which we first summarize some basic results concerning the unitary implementability of the dynamics. This is done by employing techniques different from those used so far to derive the Feynman propagator. In particular, we calculate the transition amplitudes for the usual harmonic oscillator eigenstates and define suitable semiclassical states for some physically relevant models.

We then explore the possible extension of this study to infinite dimensional dynamical systems. Specifically, we construct Schrödinger functional representations in terms of appropriate probability spaces, analyze the unitarity of the time evolution, and probe the existence of semiclassical states for a wide range of physical systems, particularly, the well-known Minkowskian free scalar fields and Gowdy cosmological models.

*Keywords:* Time dependent harmonic oscillator   Quantum field theory   Schrödinger representation

## 1. Introduction

The quantum time-dependent harmonic oscillator (TDHO) has received a lot of attention due to its usefulness to describe the dynamics of many physical systems. This is the case, for example, of radiation fields propagating outside time-dependent laser sources or in spatial regions filled with time-dependent dielectric constant matter [1]. The behavior of ions in Paul traps [2–4] can also be described by one-dimensional harmonic oscillators with time-dependent frequencies. The mathematical aspects of the quantum TDHO and its applications to more general theoretical models have been profusely analyzed in the literature [5–8]. In particular, they have been studied in the context of the search of exact invariants for nonstationary quantum systems. This method was introduced for the first time by Lewis and Riesenfeld [9,10] and proved to be especially useful to generate exact solutions to the Schrödinger equation and also to probe the existence and properties of semiclassical states for these systems.

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In the context of infinite dimensional dynamical systems, physical theoretical models with infinitely many time-dependent oscillators naturally appear in quantum field theory in curved space-times [11,12] and also in the reduced phase space description of some midisuperspace models in general relativity [13–16]. It is clear that, in the quest for a suitable quantization for these systems, the understanding of the special features of the single TDHO is particularly advisable. This fact motivates us to summarize in a rigorous and self-contained way the theory of the quantum TDHO in the first part of the paper by (implicitly) making use of the theory of invariants. Although some of the basic results such as the formula of the Feynman propagator are certainly well-known, they will be recovered by using novel techniques, and contrasted with the expressions obtained in the existing literature. This procedure will facilitate the generalization to field theories in the second part of the paper, where we apply the ideas exposed for the one-dimensional oscillator in order to obtain the propagator for infinite-dimensional systems and discuss applications both to quantum field theory and quantum gravity. The structure of the article is the following.

In Section 2, we analyze some relevant properties of the classical TDHO equation, in particular, its connection with the so-called Ermakov–Pinney (EP) equation [17–19], which plays an auxiliary role in the calculation of invariants for nonquadratic Hamiltonian systems [20]. Many of the quantities derived in this section are used afterward to obtain a simple and closed expression for the unitary evolution operator of the quantum TDHO.

In Section 3, we first briefly review the definition of the abstract Weyl  $C^*$ -algebra of quantum observables for the TDHO, the uniqueness of all regular irreducible representations of the canonical commutation relations, and the unitary implementability of the symplectic transformations that characterize the classical time evolution. Once a concrete representation is fixed, we construct the unitary evolution operator by introducing some suitable displacement and squeeze operators [21]. In our discussion, the use of the auxiliary EP equation is appropriately interpreted as a natural way to solve the Schrödinger equation and obtain an expression of the evolution operator valid for *all* values of the time parameter. We then show that this method is especially useful to derive the Feynman propagator, whose calculation follows readily in this context. We obtain an expression in agreement with those previously derived in the existing literature, where (more complicated) path-integration techniques are often employed [22,23]. We also analyze in this section the calculation of the transition amplitudes for the usual harmonic oscillator eigenstates and, as a particular case, the instability of the vacuum state as a direct consequence of the nonautonomous nature of the system.

The eigenstates of the Lewis invariant [9] provide a family of state vectors closed under time evolution, depending on a particular solution to the EP equation, that generalize the minimal wave packets of the harmonic oscillator with constant frequency. These states, however, do not have the usual properties of the ordinary coherent states—not even the ones associated with the squeezed states—and can be taken as semiclassical states just in case they are well-behaved enough. In Section 4, we analyze the construction of semiclassical states for some physically relevant systems, such as the vertically driven pendulum and, particularly, the class of TDHO equations that occur in the well-known Gowdy cosmological models [24], as a previous step to generalize this construction to field theories.

Section 5 is precisely devoted to the extension of the previous study to linear dynamical systems with infinite degrees of freedom governed by nonautonomous quantum Hamiltonians that can be interpreted as systems of infinite uncoupled harmonic oscillators with time-dependent frequencies. This fact allows us to give a straightforward procedure to obtain the unitary evolution operator, following the discussion developed for a single oscillator. We particularize our results to the well-known Minkowskian free scalar fields and also to the Gowdy cosmologies, that have attracted considerable

attention in recent years as appealing frameworks to test quantum gravity theories (see [14–16,25–27] and references therein). Making use of Schrödinger representations, where states act as functionals on appropriate quantum configuration spaces, we construct the analog of the one-dimensional propagator. We also discuss the difficulties that arise when dealing with infinite dimensional systems—specifically, the impossibility of unitarily implementing some symplectic transformations—and their implications for the search of semiclassical states. We conclude the paper with some final comments and remarks in Section 6 and Appendix A.

Throughout the paper, we will take units such that the Planck constant  $\hbar$ , the light velocity  $c$ , and the characteristic mass of the system under study are equal to one. For any  $z \in \mathbb{C} \setminus (-\infty, 0]$ ,  $\sqrt{z}$  will denote the unique square root of  $z$  such that  $\text{Re}(\sqrt{z})$  is strictly positive.

## 2. Properties of the TDHO equation

We will review in this section some properties of the classical equation of motion of a single harmonic oscillator with time-dependent frequency, from now on referred to as the TDHO equation, given by

$$\ddot{u}(t) + \kappa(t)u(t) = 0, \quad t \in I = (t_-, t_+) \subseteq \mathbb{R}, \quad (1)$$

where  $\kappa : I \rightarrow \mathbb{R}$  is a real-valued continuous function and time-derivatives are denoted by dots. Given an initial time  $t_0 \in I$ , let  $c_{t_0}$  and  $s_{t_0}$  be the independent solutions of (1) such that  $c_{t_0}(t_0) = \dot{s}_{t_0}(t_0) = 1$  and  $s_{t_0}(t_0) = \dot{c}_{t_0}(t_0) = 0$ . These can be written in terms of any set of independent solutions to (1), say  $u_1$  and  $u_2$ , as

$$c_{t_0}(t) = \frac{\dot{u}_2(t_0)u_1(t) - \dot{u}_1(t_0)u_2(t)}{W(u_1, u_2)}, \quad s_{t_0}(t) = \frac{u_1(t_0)u_2(t) - u_2(t_0)u_1(t)}{W(u_1, u_2)}, \quad (2)$$

where  $(t_0, t) \in I \times I$  and  $W(u_1, u_2) := u_1\dot{u}_2 - \dot{u}_1u_2$  denotes the (time-independent) Wronskian of  $u_1$  and  $u_2$ . In what follows, we will use the notation  $c(t, t_0) := c_{t_0}(t)$ ,  $\dot{c}(t, t_0) := \dot{c}_{t_0}(t)$ ,  $s(t, t_0) := s_{t_0}(t)$ , and  $\dot{s}(t, t_0) := \dot{s}_{t_0}(t)$ . Note that the  $s$  function belongs to the class  $C^2(I \times I)$ , whereas  $c(\cdot, t_0) \in C^2(I)$  and  $c(t, \cdot) \in C^1(I)$ . As a concrete example, for the time independent harmonic oscillator (TIHO) with constant frequency  $\kappa(t) = \kappa_0 \in \mathbb{R}$ , we simply get ( $\omega > 0$ )

$$\kappa_0 = \omega^2, \quad c(t, t_0) = \cos((t - t_0)\omega), \quad s(t, t_0) = \omega^{-1} \sin((t - t_0)\omega); \quad (3)$$

$$\kappa_0 = 0, \quad c(t, t_0) = 1, \quad s(t, t_0) = t - t_0; \quad (4)$$

$$\kappa_0 = -\omega^2, \quad c(t, t_0) = \cosh((t - t_0)\omega), \quad s(t, t_0) = \omega^{-1} \sinh((t - t_0)\omega). \quad (5)$$

In fact, as well known from Sturm's theory, the  $c$  and  $s$  functions corresponding to arbitrary frequencies share several properties with the usual cosine and sine functions. Firstly, their Wronskian is normalized to unit,  $W(c, s) = 1$ . Hence, if one of them vanishes for some time  $t = t_*$ , then the other is automatically different from zero at that instant. In view of this condition and Eq. (2), their time-derivatives satisfy

$$\dot{s}(t, t_0) = c(t_0, t), \quad \dot{c}(t, t_0) = \frac{c(t, t_0)c(t_0, t) - 1}{s(t, t_0)}, \quad (6)$$

where the last equation must be understood as a limit for those values of the time parameter  $t_*$  such that  $s(t_*, t_0) = 0$ . The odd character of the sine function translates into the condition  $s(t_0, t) = -s(t, t_0)$ . Finally, the well-known formula for the sine of a sum of angles can be generalized as

$$s(t_2, t_1) = c(t_1, t_0)s(t_2, t_0) - c(t_2, t_0)s(t_1, t_0). \quad (7)$$

It is well known that solutions to the TDHO Eq. (1) are related to certain non-linear differential equations. Here, we will restrict our attention to the so-called Ermakov–Pinney (EP) equation (see [17,18]; the interested reader is strongly suggested to consult the historical account of [19] and references therein). Let

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}$$

be a positive definite quadratic form with  $\det(A) = 1$ . Then, the (never vanishing) function  $\rho : I \rightarrow (0, +\infty)$  defined as

$$\rho(t) := \sqrt{a_{11}c^2(t, t_0) + a_{22}s^2(t, t_0) + 2a_{12}s(t, t_0)c(t, t_0)} \quad (8)$$

satisfies the EP equation

$$\ddot{\rho}(t) + \kappa(t)\rho(t) = \frac{1}{\rho^3(t)}, \quad t \in I. \quad (9)$$

According to Eq. (2), the most general analytic solution to Eq. (9) can be written as [28,29]

$$\rho(t) = \sqrt{b_{11}u_1^2(t) + b_{22}u_2^2(t) + 2b_{12}u_1(t)u_2(t)}, \quad (10)$$

where, as a consequence of (8) and (9), the coefficients  $b_{11}, b_{12}, b_{22} \in \mathbb{R}$  satisfy  $W^2(u_1, u_2) = (b_{11}b_{22} - b_{12}^2)^{-1} > 0$ . Conversely, given any solution to the EP equation it is possible to find the general solution to the TDHO equation. Indeed, it is straightforward to prove the following theorem.

**Theorem 1.** *Let  $\rho$  be any solution to the EP Eq. (9); then, the  $c$  and  $s$  solutions to (1) are given by*

$$c(t, t_0) = \frac{\rho(t)}{\rho(t_0)} \cos\left(\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right) - \rho(t)\dot{\rho}(t_0) \sin\left(\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right), \quad (11)$$

$$s(t, t_0) = \rho(t)\rho(t_0) \sin\left(\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right), \quad (t, t_0) \in I \times I. \quad (12)$$

**Remark 1.** By using Eqs. (11) and (12), it is possible to find other  $\rho$ -independent objects. For example, the combination

$$\frac{\rho(t_0)}{\rho(t)} \cos\left(\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right) + \rho(t_0)\dot{\rho}(t) \sin\left(\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right) = c(t_0, t) = \dot{s}(t, t_0)$$

and the zeros of  $s(t, t_0)$ , characterized by

$$\int_{t_0}^t \frac{d\tau}{\rho^2(\tau)} \equiv 0 \pmod{\pi},$$

are independent of the particular solution  $\rho$  to the EP equation. These results will be profusely applied along the article.

### 3. Unitary quantum time evolution

#### 3.1. General framework

The *canonical* phase space description of the classical system under consideration consists of a non-autonomous Hamiltonian system  $(I \times \Gamma, dt, \omega, H(t))$ . Here,  $\Gamma := \mathbb{R}^2$  denotes the space of Cauchy data  $(q, p)$  endowed with the usual symplectic structure  $\omega((q_1, p_1), (q_2, p_2)) := p_1q_2 - p_2q_1, \forall (q_1, p_1), (q_2, p_2) \in \Gamma$ . The triplet  $(I \times \Gamma, dt, \omega)$  then has the mathematical structure of a cosymplectic vector space (see [30] for more details). The time-dependent Hamiltonian  $H(t) : \Gamma \rightarrow \mathbb{R}, t \in I$ , is given by

$$H(t, q, p) := \frac{1}{2}(p^2 + \kappa(t)q^2). \quad (13)$$

The solution to the corresponding Hamilton equations with initial Cauchy data  $(q, p)$  at time  $t_0$  can be written down as

$$\begin{pmatrix} q_H(t, t_0) \\ p_H(t, t_0) \end{pmatrix} = \mathcal{T}_{(t, t_0)} \cdot \begin{pmatrix} q \\ p \end{pmatrix}, \quad \mathcal{T}_{(t, t_0)} := \begin{pmatrix} c(t, t_0) & s(t, t_0) \\ \dot{c}(t, t_0) & \dot{s}(t, t_0) \end{pmatrix}. \quad (14)$$

Note that the properties stated in Section 2 about the  $c$  and  $s$  solutions to the TDHO Eq. (1) guarantee that  $\mathcal{T}_{(t,t_0)} \in SL(2, \mathbb{R}) = SP(1, \mathbb{R})$  for all  $(t, t_0) \in I \times I$ , i.e., the classical time evolution is implemented by symplectic transformations.

We now formulate the quantum theory of the TDHO by defining an appropriate abstract  $C^*$ -algebra of quantum observables [31]. This algebraic approach, although being more complicated than the traditional canonical quantization for this system, will facilitate the study of field theories in subsequent sections. We first realize that, as a consequence of the linearity of  $\Gamma$ , the set of elementary classical observables can be identified with the  $\mathbb{R}$ -vector space generated by linear functionals on  $\Gamma$ . Every pair  $\lambda := (-b, a) \in \Gamma$  has an associated functional  $F_\lambda : \Gamma \rightarrow \mathbb{R}$  such that, for all  $X = (q, p) \in \Gamma$ ,  $F_\lambda(X) := \omega(\lambda, X) = aq + bp$ . In order to quantize the system, we introduce the abstract Weyl  $C^*$ -algebra of quantum observables on  $\Gamma$ ,  $\mathcal{W}(\Gamma)$ , generated by the unitary Weyl operators  $W(\lambda) = \exp(iF_\lambda)$ ,  $\lambda \in \Gamma$ , satisfying

$$W(\lambda_1)^* = W(-\lambda_1), \quad W(\lambda_1)W(\lambda_2) = \exp(i\omega(\lambda_1, \lambda_2)/2)W(\lambda_1 + \lambda_2), \quad \forall \lambda_1, \lambda_2 \in \Gamma. \quad (15)$$

According to von Neumann's uniqueness theorem [31,32], all regular irreducible representations  $\pi : \mathcal{W}(\Gamma) \rightarrow \mathcal{B}(\mathcal{H})$  of the Weyl  $C^*$ -algebra into separable Hilbert spaces  $(\mathcal{H}, \langle \cdot | \cdot \rangle)$  are unitarily equivalent. Here,  $\mathcal{B}(\mathcal{H})$  denotes the collection of bounded linear operators on  $\mathcal{H}$ . A  $*$ -homomorphism  $\pi : \mathcal{W}(\Gamma) \rightarrow \mathcal{B}(\mathcal{H})$  is said to be a regular irreducible representation if it has  $\{0\}$  and  $\mathcal{H}$  as the only closed  $\pi$ -invariant subspaces, and  $\pi(W(0, a))$  and  $\pi(W(-b, 0))$  are strongly continuous in the  $a$  and  $b$  parameters, respectively. A well-known solution is given by the Schrödinger representation  $\pi_s : \mathcal{W}(\Gamma) \rightarrow \mathcal{B}(L^2(\mathbb{R}, dq))$  into the Hilbert space  $L^2(\mathbb{R}, dq)$  where, for all pure states  $\psi \in L^2(\mathbb{R}, dq)$ ,

$$(\pi_s(W(\lambda)) \cdot \psi)(q) := \exp(-iab/2) \exp(iaq) \psi(q + b), \quad \lambda = (-b, a) \in \Gamma.$$

Thanks to the regularity condition, the usual Heisenberg algebra can be recovered in a definite sense from the Weyl  $C^*$ -algebra. The strong continuity of  $\pi_s(W(0, a))$  and  $\pi_s(W(-b, 0))$  in the real variables  $a$  and  $b$  ensures, by virtue of Stone's theorem, the existence of (unbounded) self-adjoint generators  $Q$  and  $P$  with dense domains in  $L^2(\mathbb{R}, dq)$ . In particular, the Schwartz space  $\mathcal{S}(\mathbb{R})$  of smooth rapidly decreasing functions in  $\mathbb{R}$  is a common invariant dense domain of essential self-adjointness for  $Q$  and  $P$ , where the usual Heisenberg algebra is satisfied. For all  $\psi \in \mathcal{S}(\mathbb{R})$ , we have  $(Q\psi)(q) = q\psi(q)$  and  $(P\psi)(q) = -i\psi'(q)$ , where  $\psi'$  denotes the derivative of  $\psi$ .

Another possibility is to represent the canonical commutation relations (CCR) in the space  $L^2(\mathbb{R}, d\mu_\alpha)$  where, given some  $\alpha \in \mathbb{C} \setminus \{0\}$ ,  $\mu_\alpha$  denotes the Gaussian probability measure

$$d\mu_\alpha = \frac{1}{\sqrt{2\pi}|\alpha|} \exp\left(-\frac{q^2}{2|\alpha|^2}\right) dq.$$

To each  $\alpha$  there corresponds a family of unitary transformations  $V_\alpha(\beta) : L^2(\mathbb{R}, dq) \rightarrow L^2(\mathbb{R}, d\mu_\alpha)$  connecting the standard Hilbert space with the new one in the form

$$\Psi(q) = (V_\alpha(\beta)\psi)(q) = \left(\sqrt{2\pi}|\alpha|\right)^{1/2} \exp(-i\bar{\beta}q^2/(2\bar{\alpha}))\psi(q), \quad (16)$$

where the complex numbers  $\beta$  must satisfy  $\alpha\bar{\beta} - \beta\bar{\alpha} = i$ . Note that the unitary transformations  $V_\alpha(\beta)$  map the 'vacuum' state

$$\psi_0(q) = \left(\sqrt{2\pi}|\alpha|\right)^{-1/2} \exp(i\bar{\beta}q^2/(2\bar{\alpha})) \in L^2(\mathbb{R}, dq)$$

into the unit function  $\Psi_0(q) = (V_\alpha(\beta)\psi_0)(q) = 1 \in L^2(\mathbb{R}, d\mu_\alpha)$ . In these cases, the position and momentum operators act on state vectors as

$$(Q\Psi)(q) = q\Psi(q) \quad \text{and} \quad (P\Psi)(q) = -i\Psi'(q) + \frac{\bar{\beta}}{\alpha}q\Psi(q),$$

where, with the aim of simplifying the notation,  $Q$  and  $P$  respectively denote the Schrödinger transformed operators  $V_\alpha(\beta)QV_\alpha(\beta)^{-1}$  and  $V_\alpha(\beta)PV_\alpha(\beta)^{-1}$  with common dense domain  $V_\alpha(\beta)\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, d\mu_\alpha)$ .

Any regular irreducible representation  $\pi : \mathcal{W}(\Gamma) \rightarrow \mathcal{B}(\mathcal{H})$  is stable under time evolution, i.e., there exists a (biparametric) family of unitary operators  $U(t, t_0) : \mathcal{H} \rightarrow \mathcal{H}$ , the so-called quantum time evolution operator, such that

$$U^{-1}(t, t_0) \pi(W(\lambda)) U(t, t_0) = \pi(W(\mathcal{T}_{(t, t_0)} \lambda)), \quad \forall W(\lambda) \in \mathcal{W}(\Gamma), \quad \forall (t, t_0) \in I \times I, \quad (17)$$

with  $\mathcal{T}_{(t, t_0)}$  defined in Eq. (14). These relations determine  $U(t, t_0)$  univocally up to phase. It is important to notice at this point that, if there exist singularities for the classical evolution at the boundary of the interval  $I$ , they also occur for the quantum dynamics, i.e., there is no resolution of classical singularities. On the other hand, we will check in Section 5 that the unitary implementability of symplectic transformations like those corresponding to the classical time evolution is not directly guaranteed for infinite-dimensional systems. The Heisenberg equations for  $Q$  and  $P$  can be solved just by the same expressions involved in the classical solutions (14), i.e.,

$$\begin{pmatrix} Q_H(t, t_0) \\ P_H(t, t_0) \end{pmatrix} := U^{-1}(t, t_0) \begin{pmatrix} Q \\ P \end{pmatrix} U(t, t_0) = \begin{pmatrix} c(t, t_0) & s(t, t_0) \\ \dot{c}(t, t_0) & \dot{s}(t, t_0) \end{pmatrix} \begin{pmatrix} Q \\ P \end{pmatrix}. \quad (18)$$

With more generality, given any well-behaved (analytic) classical observable  $F : \Gamma \rightarrow \mathbb{R}$  for the TDHO, the time evolution of its quantum counterpart  $F_H(t, t_0) := U^{-1}(t, t_0) F(Q, P) U(t, t_0)$  in the Heisenberg picture is simply given by

$$F_H(t, t_0) = F(Q_H(t, t_0), P_H(t, t_0)) = F(c(t, t_0)Q + s(t, t_0)P, \dot{c}(t, t_0)Q + \dot{s}(t, t_0)P). \quad (19)$$

Hence, the matrix elements  $\langle \Psi_2 | U^{-1}(t_2, t_1) F(Q, P) U(t_2, t_1) | \Psi_1 \rangle$ ,  $\Psi_1, \Psi_2 \in \mathcal{H}$ , can be computed without the explicit knowledge of the unitary evolution operator. This is also the case for the probability transitions  $\text{Prob}(\Psi_2, t_2 | \Psi_1, t_1) = |\langle \Psi_2 | U(t_2, t_1) | \Psi_1 \rangle|^2$ , as will be discussed in detail in Section 3.4. The commutators of time-evolved observables can be also calculated without the concrete expression of  $U(t_2, t_1)$ . For instance, from Eq. (19) we easily obtain

$$[Q_H(t_1, t_0), Q_H(t_2, t_0)] = i s(t_1, t_2) \mathbf{1},$$

where we have used the relation (7) stated in Section 2. As expected, the commutator given above is proportional to the identity operator and independent of the choice of the initial time  $t_0$ . Note, in contrast with the transition probabilities, that the calculation of transition amplitudes of the type  $\langle \Psi_2 | U(t_2, t_1) | \Psi_1 \rangle$  does require the explicit knowledge of (the phase of) the evolution operator. This is also the case for the (strong) derivatives of both  $U(\cdot, t_0)$  and  $U(t, \cdot)$ .

The dynamics of the quantum TDHO is governed by an (unbounded) nonautonomous Hamiltonian operator  $H(t) : \mathcal{H} \rightarrow \mathcal{H}$ ,  $t \in I$ , satisfying

$$\dot{U}(t, t_0) = -iH(t)U(t, t_0). \quad (20)$$

Given the quadratic nature of the classical Hamiltonian (13),  $H(t)$  must coincide with the operator directly promoted from the classical function modulo a  $t$ -dependent real term proportional to the identity  $\mathbf{1}$  encoding the election of  $U(t, t_0)$  satisfying Eq. (17). For a concrete representation of the CCR, we will simply take

$$H(t) := \frac{1}{2} (P^2 + \kappa(t)Q^2). \quad (21)$$

This choice fixes  $U(t, t_0)$  uniquely. The Hamiltonian (21) is a self-adjoint operator with dense domain  $\mathcal{D}_{H(t)}$ —equal to  $C_0^\infty(\mathbb{R})$  in the standard Schrödinger representation—for each value of the time parameter  $t$ . We will prove the following theorem in the next subsections.

**Theorem 2.** *The action of the unitary TDHO evolution operator  $U(t, t_0)$  corresponding to the Hamiltonian (21) on any state vector  $\psi \in \mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dq)$  in the traditional Schrödinger representation is given by*

$$(U(t, t_0)\psi)(q) = \int_{\mathbb{R}} K(q, t; q_0, t_0) \psi(q_0) dq_0,$$

where the propagator  $K(q, t; q_0, t_0)$  depends on times  $t_0$  and  $t$  through the classical TDHO solutions  $c$  and  $s$ . Explicitly,

$$K(q, t; q_0, t_0) = \frac{1}{\sqrt{2\pi i}} s^{-1/2}(t, t_0) \exp\left(\frac{i}{2s(t, t_0)}(c(t_0, t)q^2 + c(t, t_0)q_0^2 - 2qq_0)\right), \quad (22)$$

wherever  $s(t, t_0) \neq 0$ , and

$$K(q, t; q_0, t_0) = c^{-1/2}(t, t_0) \exp\left(i \frac{\dot{c}(t, t_0)}{2c(t, t_0)}\right) \delta(q_0 - q/c(t, t_0)) \quad (23)$$

if  $s(t, t_0) = 0$ .

**Remark 2.** Given a solution  $u(t)$  to the TDHO Eq. (1) which is positive in some interval  $(t_0, t_0 + \varepsilon) \subset I, \varepsilon > 0$ , we define

$$u^\epsilon(t, t_0) := \exp(i\epsilon\pi m(u; t, t_0))|u(t)|^\epsilon, \quad \epsilon \in \mathbb{R}, \quad t \in I,$$

where  $m(u; t, t_0) \in \mathbb{Z}$  is the index function of  $u$ , with  $m(u; t_0, t_0) = 0$ , defined in such a way that  $m(u; t_2, t_0) - m(u; t_1, t_0), t_1 < t_2$ , gives the number of zeros of  $u(\cdot, t_0)$  in the interval  $(t_1, t_2]$ . Finally,  $\delta(q)$  denotes the Dirac delta distribution.

**Remark 3.** Let  $\vartheta : I \rightarrow \mathbb{R}$  be a real-valued continuous function and consider the Hamiltonian

$$H_1(t) := H(t) + \vartheta(t)\mathbf{1}$$

defined in terms of (21). The unitary evolution  $U_1(t, t_0)$  associated with  $H_1(t)$  satisfying Eq. (17) gives rise to the propagator

$$K_1(q, t; q_0, t_0) = K(q, t; q_0, t_0) \exp\left(-i \int_{t_0}^t \vartheta(\tau) d\tau\right). \quad (24)$$

Note that  $U_1^{-1}(t, t_0) \mathcal{O} U_1(t, t_0) = U^{-1}(t, t_0) \mathcal{O} U(t, t_0)$  for any quantum observable  $\mathcal{O}$ .

**Remark 4.** In the  $L^2(\mathbb{R}, d\mu_x)$ -representation defined by the unitary transformation  $V_\alpha(\beta)$  (see Eq. (16)), the evolution is given by

$$(U(t, t_0)\Psi)(q) = \int_{\mathbb{R}} K_{\alpha\beta}(q, t; q_0, t_0) \Psi(q_0) d\mu_x(q_0),$$

where

$$K_{\alpha\beta}(q, t; q_0, t_0) := \sqrt{2\pi}|\alpha| \exp\left(\frac{i\beta}{2\alpha}q_0^2 - \frac{i\bar{\beta}}{2\bar{\alpha}}q^2\right) K(q, t; q_0, t_0). \quad (25)$$

### 3.2. Constructing the evolution operator

In order to calculate the unitary evolution operator  $U(t, t_0)$  we will perform a generalization of the method developed in [21] that will clarify the appearance of the auxiliary Ermakov–Pinney solution (10) in this context, and will allow us also to warn the reader about other problematic choices that have appeared before in the related literature. We first introduce on  $\mathcal{H}$  the (one-parameter family of) unitary operators

$$D(x) := \exp\left(-\frac{i}{2}xQ^2\right), \quad x \in \mathbb{R},$$

generating a displacement of the momentum operator,  $D(x)PD^{-1}(x) = P + xQ$  (the position operator being unaffected by them), and define the unitary squeeze operators

$$S(y) := \exp\left(\frac{i}{2}y(QP + PQ)\right), \quad y \in \mathbb{R},$$



scaling both the position and momentum operator as  $S(y)QS^{-1}(y) = e^yQ$  and  $S(y)PS^{-1}(y) = e^{-y}P$ , respectively. Let  $\Psi(t) \in \mathcal{D}_{H(t)}$ ,  $t \in I$ , be a solution to the Schrödinger equation, i.e.,  $i\dot{\Psi}(t) = H(t)\Psi(t)$ , and let  $x, y \in C^1(I)$ . We now introduce the unitary operators

$$T(t) = T(t; x, y) := S(y(t))D(x(t)),$$

where the functions  $x$  and  $y$  remain arbitrary at this stage. Let us consider the time evolution for the transformed state vector

$$\Phi(t) = \Phi(t; x, y) := T(t; x, y)\Psi(t),$$

given by

$$\begin{aligned} i\dot{\Phi}(t) &= \left( T(t)H(t)T^{-1}(t) - iT(t)\dot{T}(t) \right) \Phi(t) \\ &= \frac{1}{2} \left( e^{-2y(t)}P^2 + (x(t) - \dot{y}(t))(QP + PQ) + e^{2y(t)}(x^2(t) + \kappa(t) + \dot{x}(t))Q^2 \right) \Phi(t). \end{aligned}$$

We note at this point that it is possible to get a notable simplification of the previous expression just by imposing

$$x(t) = \dot{y}(t) \quad \text{and} \quad x^2(t) + \kappa(t) + \dot{x}(t) = \exp(-4y(t)). \quad (26)$$

The most natural way to achieve this is to choose

$$y(t) := \log \rho(t) \quad \text{and, hence,} \quad x(t) = \dot{\rho}(t)/\rho(t),$$

with  $\rho$  being any solution to the auxiliary EP Eq. (9) introduced in Section 2. In this way, the state vector  $\Phi(t; \dot{\rho}/\rho, \log \rho) =: \Phi_\rho(t)$  satisfies the differential equation

$$i\dot{\Phi}_\rho(t) = \frac{1}{2\rho^2(t)} (P^2 + Q^2) \Phi_\rho(t).$$

Solving this equation and going back to the original state vector  $\Psi(t)$ , we finally obtain the unitary evolution operator for the system. We can then enunciate the following theorem.

**Theorem 3.** *The time evolution operator  $U(t, t_0)$  for the quantum TDHO whose dynamics is governed by the Hamiltonian (21) is given by a composition of unitary operators*

$$U(t, t_0) = T_\rho^{-1}(t)R_\rho(t, t_0)T_\rho(t_0),$$

where

$$R_\rho(t, t_0) := \exp \left( -\frac{i}{2} \int_{t_0}^t \frac{d\tau}{\rho^2(\tau)} (P^2 + Q^2) \right), \quad (27)$$

and  $T_\rho(t) = S_\rho(t)D_\rho(t)$ , with

$$D_\rho(t) := \exp \left( -\frac{i}{2} \frac{\dot{\rho}(t)}{\rho(t)} Q^2 \right) \quad \text{and} \quad S_\rho(t) := \exp \left( \frac{i}{2} \log \rho(t) (QP + PQ) \right). \quad (28)$$

**Remark 5.** Note that instead of introducing  $\rho$ , we could have used other choices for the  $x$  and  $y$  functions. In these cases, conditions (26) may not hold and the expressions of the evolution operator would differ from the one obtained here. For instance, one can select  $x(t) = \dot{u}(t)/u(t)$  and  $y(t) = \log u(t)$  as in [21], with  $u(t)$  being any solution to the TDHO equation, but this choice is problematic because the set  $\{t \in I \mid u(t) = 0\}$  must be non-empty and, hence, the resulting formula for the unitary operator is generally not well-defined for all values of the time parameter  $t$ . This is the reason why the election of the Ermakov–Pinney solution is especially convenient in this context—recall that  $\rho$  is a positive definite function. It follows from the above that the appearance of this solution is nearly unavoidable in this context.

Note that the eigenstates of the  $R_\rho(t, t_0)$  operator (27) are given by those of the Hamiltonian operator corresponding to a quantum harmonic oscillator with unit frequency  $\sqrt{\kappa(t)} = 1$ ,

$$H_0 := \frac{1}{2} (P^2 + Q^2). \quad (29)$$

This fact will be shown to be particularly useful to calculate the Feynman propagator. It is also important to point out that the procedure employed in this section is implicitly based upon the transformation of the so-called Lewis invariant [9]

$$I_\rho(t) := \frac{1}{2} \left( \frac{Q^2}{\rho^2(t)} + (\rho(t)P - \dot{\rho}(t)Q)^2 \right), \quad \dot{I}_{\rho_H} = 0, \quad (30)$$

into an explicitly time-independent quantity—although in order to obtain the unitary operator it has not been necessary to use it. In this case, we simply have

$$T_\rho(t)I_\rho(t)T_\rho^{-1}(t) = H_0. \quad (31)$$

The Lewis invariant is often used to generate exact solutions to the Schrödinger equation, and turns out to be especially useful to construct semiclassical states for these systems, as will be discussed later.

### 3.3. Propagator formula

We finally proceed to derive the Feynman propagator for the quantum TDHO corresponding to the Hamiltonian (21). In the previous subsection, we have written down the evolution operator for this system explicitly in closed form in terms of the position and momentum operators (see Theorem 3). It is given by the product of the unitary operators (27) and (28). We calculate now the action of these factors on test functions  $\psi \in \mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}, dq)$  in the standard Schrödinger representation. First, it is straightforward to see that

$$\begin{aligned} (T_\rho(t)\psi)(q) &= \sqrt{\rho(t)} \exp\left(-\frac{i}{2}\dot{\rho}(t)\rho(t)q^2\right) \psi(\rho(t)q) = \int_{\mathbb{R}} K_\rho^+(q, t; q_0) \psi(q_0) dq_0, \\ (T_\rho^{-1}(t)\psi)(q) &= \frac{1}{\sqrt{\rho(t)}} \exp\left(\frac{i}{2}\frac{\dot{\rho}(t)}{\rho(t)}q^2\right) \psi(q/\rho(t)) = \int_{\mathbb{R}} K_\rho^-(q, t; q_0) \psi(q_0) dq_0, \end{aligned}$$

where we have introduced the distributions

$$K_\rho^+(q, t; q_0) := \sqrt{\rho(t)} \exp\left(-\frac{i}{2}\dot{\rho}(t)\rho(t)q^2\right) \delta(q_0 - \rho(t)q), \quad (32)$$

$$K_\rho^-(q, t; q_0) := \frac{1}{\sqrt{\rho(t)}} \exp\left(\frac{i}{2}\frac{\dot{\rho}(t)}{\rho(t)}q^2\right) \delta(q_0 - q/\rho(t)). \quad (33)$$

The propagator for  $R_\rho(t, t_0)$ , satisfying

$$(R_\rho(t, t_0)\psi)(q) = \int_{\mathbb{R}} K_\rho^0(q, t; q_0, t_0) \psi(q_0) dq_0,$$

can be easily derived from the one corresponding to the TIHO with unit frequency. As is well known [33,34], the Green function  $K^0$  for the Hamiltonian (29) is given by the Feynman–Soriau formulae

$$\begin{aligned} K^0(q, v; q_0, 0) &= \frac{1}{\sqrt{2\pi i}} \sin^{-1/2}(v, 0) \exp\left(\frac{i}{2\sin v}((q^2 + q_0^2) \cos v - 2qq_0)\right), \quad v \not\equiv 0 \pmod{\pi}, \\ K^0(q, v; q_0, 0) &= \cos^{-1/2}(v, 0) \exp\left(-\frac{i \sin v}{2 \cos v}\right) \delta(q_0 - q/\cos v), \quad v \equiv 0 \pmod{\pi}, \end{aligned}$$

where the so-called Maslov correction factor [34], which allows the calculation of the propagator beyond the caustics  $\{v \in \mathbb{R} : \sin(v) = 0\} = \{\pi k : k \in \mathbb{Z}\}$ , has been conveniently absorbed into the definition of  $\sin^{1/2}(v, 0)$  and  $\cos^{1/2}(v, 0)$  given in the formulation of Theorem 2. In view of Eq. (27), we simply get

$$K_{\rho}^0(q, t; q_0, t_0) = K^0\left(q, \int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}; q_0, 0\right). \quad (34)$$

Therefore,

$$(U(t, t_0)\psi)(q) = \left(T_{\rho}^{-1}(t)R_{\rho}(t, t_0)T_{\rho}(t_0)\psi\right)(q) = \int_{\mathbb{R}} K(q, t; q_0, t_0)\psi(q_0) dq_0,$$

where

$$K(q, t; q_0, t_0) = \int_{\mathbb{R}^2} K_{\rho}^{-}(q, t; q_2) K_{\rho}^0(q_2, t; q_1, t_0) K_{\rho}^{+}(q_1, t_0; q_0) dq_1 dq_2. \quad (35)$$

By combining (32)–(35) with (11) and (12), we find the formula for the propagator (22) enunciated in Theorem 2 expressed in terms of the  $c$  and  $s$  solutions to the classical TDHO equations (1). As expected, the propagator—and hence the evolution operator itself—does not depend on the particular solution  $\rho$  to the EP Eq. (9) chosen to factorize  $U(t, t_0)$ . Taking the appropriate limits one obtains, after straightforward calculations, the propagator evaluated at caustics (23). The resulting expressions are in agreement with those obtained by other authors (see, for example, [22,23,34,35]), though in our case they have been attained within a different scheme, based essentially on the previous obtention of a closed expression for the evolution operator. Finally, a direct calculation shows that the propagator  $K(q, t; q_0, t_0)$ , viewed as a function of  $(q, t)$ , formally satisfies the evolution equation

$$i\partial_t K = -\frac{1}{2}\partial_q^2 K + \frac{1}{2}q^2 \kappa(t) K.$$

### 3.4. Transition amplitudes and vacuum instability

The exact expressions for the Green functions (22) and (23) can be used to *exactly* compute both transition amplitudes and probabilities. Here, we will restrict ourselves to the class of normalized states  $\Phi_n^{\omega}$  defined in  $L^2(\mathbb{R}, dq)$  as

$$\Phi_n^{\omega}(q) := \frac{\omega^{1/4}}{\sqrt{2^n n! \sqrt{\pi}}} \exp(-\omega q^2/2) H_n(\sqrt{\omega} q), \quad \omega > 0, \quad n \in \mathbb{N}_0, \quad (36)$$

with  $H_n(z)$  denoting the  $n$ th Hermite polynomial in the variable  $z$ . Note that for any fixed value  $\omega$  the set  $(\Phi_n^{\omega} : n \in \mathbb{N}_0)$  defines the usual orthonormal basis of  $L^2(\mathbb{R})$  constituted by the eigenvectors of the quantum Hamiltonian (21) corresponding to a TIHO of constant frequency  $\sqrt{\kappa(t)} = \omega$ . Since the  $\Phi_n^{\omega}$  states are complete, the corresponding transition amplitudes and probabilities for other states are readily obtainable. By using the generating function for Hermite polynomials,

$$\exp(2\sqrt{\omega}qx - x^2) = \sum_{n=0}^{\infty} H_n(\sqrt{\omega}q) \frac{x^n}{n!},$$

it is clear that

$$\left\langle \Phi_{n_2}^{\omega_2} | U(t_2, t_1) \Phi_{n_1}^{\omega_1} \right\rangle = \frac{1}{\pi} \left( \frac{n_1! n_2! \sqrt{\omega_1 \omega_2}}{2^{n_1+n_2+1} i} \right)^{1/2} s^{-1/2}(t_2, t_1) [x_1^{n_1} x_2^{n_2}] I(x_1, x_2; A(t_1, t_2; \omega_1, \omega_2)), \quad (37)$$

where  $[x_1^{n_1} x_2^{n_2}] f(x_1, x_2)$  denotes the complex coefficient appearing in the  $x_1^{n_1} x_2^{n_2}$ -term of the Taylor expansion of function  $f$ . Here, for any matrix  $A \in \text{Mat}_{2 \times 2}(\mathbb{C})$ , we define

$$\begin{aligned} I(x_1, x_2; A) &:= \exp(-(x_1^2 + x_2^2)) \int_{\mathbb{R}^2} \exp\left(-\frac{1}{2} \vec{q}^t A \vec{q} + 2\vec{x}^t \text{diag}(\sqrt{\omega_1}, \sqrt{\omega_2}) \vec{q}\right) d^2 \vec{q} \\ &= \frac{2\pi}{\sqrt{\det A}} \exp\left(\vec{x}^t \left(2\text{diag}(\sqrt{\omega_1}, \sqrt{\omega_2}) A^{-1} \text{diag}(\sqrt{\omega_1}, \sqrt{\omega_2}) - \mathbb{I}\right) \vec{x}\right), \end{aligned}$$

whenever  $\text{Re}(A) \geq 0$  and  $\det A \neq 0$ . In this formula,  $\vec{x}$  denotes the column vector with first and second components given by  $x_1$  and  $x_2$ , respectively; we define  $\vec{q}$  similarly. In our case,

$$A(t_1, t_2; \omega_1, \omega_2) := \begin{pmatrix} \omega_1 - i \frac{c(t_2, t_1)}{s(t_2, t_1)} & \frac{i}{s(t_2, t_1)} \\ \frac{i}{s(t_2, t_1)} & \omega_2 - i \frac{c(t_1, t_2)}{s(t_2, t_1)} \end{pmatrix},$$

with

$$\det A(t_1, t_2; \omega_1, \omega_2) = \left( \omega_1 \omega_2 - \frac{\dot{c}(t_2, t_1)}{s(t_2, t_1)} \right) - i \left( \frac{\omega_1 c(t_1, t_2) + \omega_2 c(t_2, t_1)}{s(t_2, t_1)} \right).$$

Here,  $\text{Re}(A(t_0, t; \omega_1, \omega_2)) \geq 0$  and  $\det A(t_0, t; \omega_1, \omega_2) \neq 0$  for all  $(t_0, t) \in I \times I$  and  $\omega_1, \omega_2 \in (0, +\infty)$ . The Taylor expansion of  $I(x_1, x_2; A)$  can be efficiently computed by applying the following lemma, that trivially follows from the multinomial formula.

**Lemma 1.** *Let*

$$B = B^t = \begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix} \in \text{Mat}_{2 \times 2}(\mathbb{C}).$$

Then, using the notation introduced above, we have

$$[x_1^{n_1} x_2^{n_2}] \exp(\vec{x}^t B \vec{x}) = b_{11}^{(n_1 - n_2)/2} (2b_{12})^{n_2} \sum_{m \in \Delta(n_1, n_2)} \frac{(b_{11} b_{22})^m (4b_{12}^2)^{-m}}{m! (m + (n_1 - n_2)/2)! (n_2 - 2m)!},$$

whenever  $n_1$  and  $n_2$  have the same parity, and vanishes otherwise. Here,  $\Delta(n_1, n_2) := \{m \in \mathbb{N}_0 : \max\{0, (n_2 - n_1)/2\} \leq m \leq \lfloor n_2/2 \rfloor\}$ , where  $\lfloor x \rfloor$  denotes the largest integer less than or equal to  $x \in \mathbb{R}$ . In particular, taking  $n_1 = 0$ , we get

$$[x_1^0 x_2^{n_2}] \exp(\vec{x}^t B \vec{x}) = \frac{b_{22}^{n_2/2}}{(n_2/2)!} \quad \text{for } n_2 \equiv 0 \pmod{2}, \quad (38)$$

and vanishes when  $n_2$  is an odd number.

**Remarks.** Note that the TDHO quantum dynamics is invariant under parity inversion  $\mathbf{P}$  and the states  $\phi_n^\omega$  satisfy  $\mathbf{P} \phi_n^\omega = (-1)^n \phi_n^\omega$ . Hence,  $\langle \phi_{n_2}^{\omega_2} | U(t_2, t_1) \phi_{n_1}^{\omega_1} \rangle = 0$  if  $n_1$  and  $n_2$  have different parity.

As a concrete example, in the case of a TIHO with constant frequency  $\omega = \omega_1 = \omega_2$ , we identify

$$B = 2 \text{diag}(\sqrt{\omega}, \sqrt{\omega}) A^{-1}(t_1, t_2; \omega, \omega) \text{diag}(\sqrt{\omega}, \sqrt{\omega}) - \mathbb{I} = \exp(-i\omega(t_2 - t_1)) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and, hence,

$$I(x_1, x_2; A(t_1, t_2; \omega, \omega)) = \sum_{n=0}^{\infty} \frac{2^n}{n!} \exp(-i\omega n(t_2 - t_1)) x_1^n x_2^n.$$

This is in perfect agreement with

$$\langle \phi_{n_2}^\omega | U(t_2, t_1) \phi_{n_1}^\omega \rangle = \exp(-i\omega(n_1 + 1/2)(t_2 - t_1)) \delta(n_1, n_2),$$

where  $\delta(n_1, n_2)$  denotes the Kronecker delta. For arbitrary time-dependent frequencies the formula (37), when restricted to the same initial and final frequencies  $\omega_1 = \omega_2$ , coincides with the one given in [36] written in terms of associated Legendre functions.

We conclude this section with the analysis of the instability of the vacuum state  $\phi_0^\omega$  due to the non-autonomous nature of the Hamiltonian (21). This can be easily derived from the formulae (37) and (38).

**Theorem 4.** *The quantum time evolution of the vacuum state  $\Phi_0^\omega$  is generally given by a superposition of states  $U(t, t_0) \Phi_0^\omega = \sum_{n \in \mathbb{N}_0} \langle \Phi_{2n}^\omega | U(t, t_0) \Phi_0^\omega \rangle \Phi_{2n}^\omega$ , where the probability amplitudes  $\langle \Phi_{2n}^\omega | U(t, t_0) \Phi_0^\omega \rangle$  are given by*

$$\langle \Phi_{2n}^\omega | U(t, t_0) \Phi_0^\omega \rangle = \frac{\sqrt{(2n)!}}{2^n n!} \left( 2\omega (A^{-1}(t_0, t; \omega, \omega))_{22} - 1 \right)^n \langle \Phi_0^\omega | U(t, t_0) \Phi_0^\omega \rangle, \quad n \in \mathbb{N}, \quad (39)$$

in terms of the expectation value

$$\langle \Phi_0^\omega | U(t, t_0) \Phi_0^\omega \rangle = \sqrt{\frac{2\omega}{\det \Lambda(t_0, t; \omega, \omega)}} \exp(-i\pi/4) s^{-1/2}(t, t_0),$$

with

$$(\Lambda^{-1}(t_0, t; \omega, \omega))_{22} = \frac{\omega s^2(t_2, t_1) - is(t_2, t_1)c(t_2, t_1)}{1 + \omega^2 s^2(t_2, t_1) - c(t_2, t_1)c(t_1, t_2) - i\omega s(t_2, t_1)(c(t_2, t_1) + c(t_1, t_2))}.$$

**Remarks.** Consider the usual annihilation and creation operators

$$a_\omega := \frac{1}{\sqrt{2}}(\sqrt{\omega}Q + iP/\sqrt{\omega}) \quad \text{and} \quad a_\omega^* := \frac{1}{\sqrt{2}}(\sqrt{\omega}Q - iP/\sqrt{\omega}), \quad (40)$$

with  $[a_\omega, a_\omega^*] = \mathbf{1}$  and  $[a_\omega, a_\omega] = 0 = [a_\omega^*, a_\omega^*]$ , such that  $a_\omega^* \Phi_n^\omega = \sqrt{n+1} \Phi_{n+1}^\omega$  and  $a_\omega \Phi_n^\omega = \sqrt{n} \Phi_{n-1}^\omega, \forall n \in \mathbb{N}$ , with  $a_\omega \Phi_0^\omega = 0$ . The evolution of these operators in the Heisenberg picture can be obtained directly from Eq. (18),

$$\begin{aligned} U^{-1}(t, t_0) a_\omega U(t, t_0) &= A_\omega(t, t_0) a_\omega + B_\omega(t, t_0) a_\omega^*, \\ U^{-1}(t, t_0) a_\omega^* U(t, t_0) &= \bar{B}_\omega(t, t_0) a_\omega + \bar{A}_\omega(t, t_0) a_\omega^*, \end{aligned} \quad (41)$$

where  $A_\omega(t, t_0)$  and  $B_\omega(t, t_0)$  are the Bogoliubov coefficients

$$A_\omega(t, t_0) := \frac{1}{2} (c(t, t_0) + \dot{s}(t, t_0) + i(\omega^{-1} \dot{c}(t, t_0) - \omega s(t, t_0))), \quad (42)$$

$$B_\omega(t, t_0) := \frac{1}{2} (c(t, t_0) - \dot{s}(t, t_0) + i(\omega^{-1} \dot{c}(t, t_0) + \omega s(t, t_0))), \quad (43)$$

satisfying  $A_\omega(t, t_0) = \bar{A}_\omega(t_0, t)$ ,  $B_\omega(t, t_0) = -B_\omega(t_0, t)$ , and  $|A_\omega(t, t_0)|^2 - |B_\omega(t, t_0)|^2 = 1, \forall (t, t_0) \in I \times I$ . Note, in particular, that  $A_\omega(t, t_0)$  never vanishes. For example, for the TIHO of constant frequency  $\omega > 0$  we have  $B_\omega(t, t_0) = 0$  and  $A_\omega(t, t_0) = \exp(-i(t - t_0)\omega)$ . A straightforward calculation yields (see also [37] and [38])

$$U(t, t_0) \Phi_0^\omega = \langle \Phi_0^\omega | U(t, t_0) \Phi_0^\omega \rangle \exp\left(-\frac{1}{2} \frac{B_\omega(t_0, t)}{A_\omega(t_0, t)} a_\omega^2\right) \Phi_0^\omega, \quad (44)$$

This formula is in perfect agreement with the transitions (39). Indeed, it is straightforward to check that

$$2\omega(\Lambda^{-1}(t_0, t; \omega, \omega))_{22} - 1 = -B_\omega(t_0, t)/A_\omega(t_0, t).$$

Since  $\det \Lambda(t_0, t; \omega, \omega) = -2i\omega s^{-1}(t, t_0)A_\omega(t_0, t)$ , the expectation value  $\langle \Phi_0^\omega | U(t, t_0) \Phi_0^\omega \rangle$  can be rewritten as

$$\langle \Phi_0^\omega | U(t, t_0) \Phi_0^\omega \rangle = \frac{1}{\sqrt{|A_\omega(t_0, t)|}} \exp(i\sigma(t, t_0)), \quad (45)$$

where the phase  $\sigma(t, t_0) \in C^1(I \times I)$  comes from a careful calculation of the principal argument. For a TIHO with constant frequency  $\omega > 0$ , we have  $\sigma(t, t_0) = (t_0 - t)\omega/2$  for all  $t, t_0 \in \mathbb{R}$ . Given an arbitrary squared frequency  $\kappa(t)$ , the phase  $\sigma(t, t_0)$  evaluated at times  $t$  close to  $t_0$  is simply given by

$$\sigma(t, t_0) = -\frac{1}{2} \arctan\left(\frac{\omega s(t, t_0) - \omega^{-1} \dot{c}(t, t_0)}{c(t, t_0) + \dot{s}(t, t_0)}\right). \quad (46)$$

The  $\sigma$  phase can be conveniently canceled through a suitable redefinition of the Hamiltonian (21) just in the case when  $\dot{\sigma}(t, t_0)$  is independent of  $t_0$ . In that situation, by identifying  $\vartheta(t) = \dot{\sigma}(t, t_0)$  in Eq. (24), we have that the redefined evolution operator satisfies  $\langle \Phi_0^\omega | U_1(t, t_0) \Phi_0^\omega \rangle = 1/\sqrt{|A_\omega(t_0, t)|}$ . In the TIHO case, we get  $\vartheta(t) = -\omega/2$  (this amounts to considering normal order). In general, it is not possible to proceed in this way in all situations when dealing with arbitrary time-dependent frequencies. In any case, the  $\sigma$  phase is irrelevant for the calculation of transition probabilities. In particular, given  $\Psi_1, \Psi_2 \in \mathcal{H}$  with  $\Psi_1 = F_1(a_\omega, a_\omega^*) \Phi_0^\omega$ , where  $F_1$  is some analytic function, we have

$$\begin{aligned} \text{Prob}(\Psi_2, t_2 | \Psi_1, t_1) &= |\langle \Psi_2 | U(t_2, t_1) \Psi_1 \rangle|^2 \\ &= \frac{|\langle \Psi_2 | F_1(a_{\omega H}(t_1, t_2), a_{\omega H}^*(t_1, t_2)) \exp(-B_{\omega}(t_1, t_2)/(2A_{\omega}(t_1, t_2))a_{\omega}^2)\Phi_0^\omega \rangle|^2}{|A_{\omega}(t_1, t_2)|}, \end{aligned}$$

where the time dependence only appears through the Bogoliubov coefficients (42) and (43). Finally, it is important to point out that the transformations (41) and the evolution of the vacuum state (44) fully characterize the quantum time evolution of the TDHO. By using these relations, we can easily compute the action of  $U(t, t_0)$  on any basic vector  $\Phi_n^\omega = \left(1/\sqrt{n!}\right) a_{\omega}^{*n} \Phi_0^\omega$ .

#### 4. Semiclassical states

In this section, we will look for states that behave semiclassically under the dynamics defined by the quantum Hamiltonian (21). We will base our study on the concrete factorization of the evolution operator defined in Theorem 3. To achieve this goal, note that the eigenvalue problem for the Lewis invariant (30) can be exactly solved. Indeed, let us fix  $t_0 \in I$  and let  $(\Phi_n : n \in \mathbb{N}_0)$  be the eigenstates (36) of the auxiliary Hamiltonian  $H_0$  (29) corresponding to unit frequency  $\omega = 1$ . According to relation (31), the initial states  $\psi_n^\rho(t_0) := T_\rho^{-1}(t_0)\Phi_n$ ,

$$\psi_n^\rho(t_0, q) = \left( \frac{1}{2^n n! \sqrt{\pi} \rho(t_0)} \right)^{1/2} \exp\left( \frac{i}{2} \left( \frac{\dot{\rho}(t_0)}{\rho(t_0)} + \frac{i}{\rho^2(t_0)} \right) q^2 \right) H_n(q/\rho(t_0)) \in L^2(\mathbb{R}, dq),$$

labeled both by  $\rho$  and the integers  $n \in \mathbb{N}_0$ , are eigenstates of  $I_\rho(t_0)$  with eigenvalues equal to  $n + 1/2$ . Consider now the initial pure state

$$\Phi_\rho^{(z)}(t_0) := T_\rho^{-1}(t_0)\Phi^{(z)} = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \psi_n^\rho(t_0), \quad z \in \mathbb{C}, \quad (47)$$

with  $\Phi^{(z)} := e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \Phi_n$  being the well-known coherent states for the Hamiltonian  $H_0$ . Let us take the annihilation and creation operators  $a$  and  $a^*$  for unit frequency  $\omega = 1$  defined in Eq. (40). The superposition (47) is a normalized eigenvector of the (time-dependent) annihilation operator

$$a_\rho(t_0) := T_\rho^{-1}(t_0) a T_\rho(t_0) = \frac{1}{\sqrt{2}} (Q/\rho(t_0) + i(\rho(t_0)P - \dot{\rho}(t_0)Q)), \quad (48)$$

in the sense that  $a_\rho(t_0)\Phi_\rho^{(z)}(t_0) = z\Phi_\rho^{(z)}(t_0)$ . This operator, together with the associated creation operator

$$a_\rho^*(t_0) := T_\rho^{-1}(t_0) a^* T_\rho(t_0) = \frac{1}{\sqrt{2}} (Q/\rho(t_0) - i(\rho(t_0)P - \dot{\rho}(t_0)Q)),$$

satisfies the Heisenberg algebra,  $[a_\rho(t_0), a_\rho^*(t_0)] = \mathbf{1}$  and  $[a_\rho(t_0), a_\rho(t_0)] = 0 = [a_\rho^*(t_0), a_\rho^*(t_0)]$ , for each initial value of the time parameter  $t_0$ . In particular, the Lewis invariant (30) may be expressed in terms of these operators as  $I_\rho(t_0) = a_\rho^*(t_0)a_\rho(t_0) + (1/2)\mathbf{1}$ . Through unitary time evolution, we get

$$\Phi_\rho^{(z)}(t, t_0) := U(t, t_0)\Phi_\rho^{(z)}(t_0) = \exp\left(-\frac{i}{2} \int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right) \Phi_\rho^{(z_\rho(t, t_0))}(t), \quad (49)$$

where we have denoted

$$z_\rho(t, t_0) := \exp\left(-i \int_{t_0}^t \frac{d\tau}{\rho^2(\tau)}\right) z, \quad z \in \mathbb{C}.$$

We want to remark that the time-dependent phase appearing in Eq. (49) is necessary for these states to verify the Schrödinger equation. In our case, they coincide with those defined in Eq. (4.6) of reference [39]. We conclude that the family of states (47) is closed under the dynamics. Moreover, the following theorem can be used to justify that these states can be considered as semiclassical under certain assumptions.

**Theorem 5.** Let  $z = x + iy \in \mathbb{C}$  and  $t_0 \in I$ . The position and momentum expectation values in the state  $\Phi_\rho^{(z)}(t, t_0) = U(t, t_0)\Phi_\rho^{(z)}(t_0)$  satisfy

$$\begin{aligned} q_H(t, t_0) &= \left\langle \Phi_\rho^{(z)}(t, t_0) \left| Q \Phi_\rho^{(z)}(t, t_0) \right\rangle = \sqrt{2} \rho(t) \operatorname{Re}(z_\rho(t, t_0)), \\ p_H(t, t_0) &= \left\langle \Phi_\rho^{(z)}(t, t_0) \left| P \Phi_\rho^{(z)}(t, t_0) \right\rangle = \sqrt{2} \operatorname{Re}((\dot{\rho}(t) - i/\rho(t))z_\rho(t, t_0)), \end{aligned}$$

where  $(q_H, p_H)$  is the classical solution (14) determined by the Cauchy data  $(q, p) = (\sqrt{2}\rho(t_0)x, \sqrt{2}(\dot{\rho}(t_0)x + y/\rho(t_0)))$  at time  $t_0$ . Moreover, the mean square deviations of the position and momentum operators with respect to the evolved state  $\Phi_\rho^{(z)}(t, t_0)$ ,

$$\Delta_{\Phi_\rho^{(z)}(t, t_0)} Q = \frac{1}{\sqrt{2}} \rho(t), \quad \Delta_{\Phi_\rho^{(z)}(t, t_0)} P = \frac{1}{\sqrt{2}} |\dot{\rho}(t) - i\rho^{-1}(t)|, \quad (50)$$

are independent of both  $t_0$  and the Cauchy data defined by  $z$ .

**Remark 6.** Given any observable  $\mathcal{O}$ , its uncertainty in the state  $\Psi \in \mathcal{D}_\mathcal{O}$  is defined as  $\Delta_\Psi \mathcal{O} := (\langle \Psi | \mathcal{O}^2 \Psi \rangle - \langle \Psi | \mathcal{O} \Psi \rangle^2)^{1/2}$ . Note that, in general, the elements of the family of states under consideration are neither standard coherent states nor squeezed states. For instance, for the free particle (4) one can choose  $\rho(t) = \sqrt{1 + (t - t_0)^2}$  and, hence,  $\Delta_{\Phi_\rho^{(z)}(t, t_0)} Q \sim t/\sqrt{2}$  for large values of  $t$ ; similar results occur for other elections of  $\rho$ . Nevertheless, it is obvious that we will obtain good semiclassical states for a system whenever the solution  $\rho$  to the auxiliary EP Eq. (9) has a suitable behavior, for instance, if  $\rho$  is periodic in time or is simply a bounded function. We will analyze some clarifying examples in this respect.

**Example 1.** (Vertically driven pendulum). Consider the vertically driven pendulum [40], i.e., the motion of a physical pendulum whose supporting point oscillates in the vertical direction. In the small angles regime, it is described by the Mathieu equation in its canonical form [41]

$$\ddot{u}(t) + \kappa(t; a, b)u(t) = 0, \quad \kappa(t; a, b) := a - 2b \cos(2t), \quad a, b \in \mathbb{R}.$$

The general solution to this equation is a real linear combination of the so-called Mathieu cosine and sine functions [42, 43], denoted respectively as  $Ce(t; a, b)$  and  $Se(t; a, b)$ . Given a nonzero  $b$  value, it is a well-known fact that the Mathieu cosine and sine functions are periodic in the time parameter  $t$  only for certain (countable number of) values of the  $a$  parameter, called *characteristic values*. The procedure to calculate these characteristic values for even or odd Mathieu functions with *characteristic exponent*<sup>1</sup>  $r \in \mathbb{Z}$  and parameter  $b$  can be efficiently implemented in a computer. In this case, solutions to the EP Eq. (9) inherit the periodic behavior from the Mathieu solutions, in such a way that one obtains well-behaved semiclassical states for which the average position and momentum follow the classical trajectories, whereas the corresponding uncertainties vary periodically in time. Note that, for small values of the  $b$  parameter, we have  $Ce(t; a, b) \sim \cos(\sqrt{a}t)$  and  $Se(t; a, b) \sim \sin(\sqrt{a}t)$ , and the system closely approximates the TIHO with squared frequency given by the  $a$  parameter.

**Example 2.** ( $\mathbb{T}^3$  Gowdy-like oscillator). Consider the TDHO equation

$$\ddot{u}(t) + \kappa(t; \omega)u(t) = 0, \quad \kappa(t; \omega) := \omega^2 + \frac{1}{4t^2}, \quad \omega \in \mathbb{R}, \quad t \in (0, +\infty).$$

This equation is satisfied for each mode of the scalar fields encoding the information about the gravitational local degrees of freedom of the so-called  $\mathbb{T}^3$  Gowdy models, which are symmetry reductions of general relativity with cosmological interpretation that admit an exact—i.e., nonperturbative—quantization (see next section). In terms of the zero Bessel functions of first and second kind [43], denoted  $J_0$  and  $Y_0$  respectively, the  $c$  and  $s$  solutions introduced in Section 2 are given by

<sup>1</sup> All Mathieu functions have the form  $\exp(ir t)F(t)$ , where  $r$  is the characteristic exponent and function  $F(t)$  has period  $2\pi$ .

$$\begin{aligned}
c(t, t_0) &= \frac{\pi}{4} \left( \sqrt{\frac{t}{t_0}} Y_0(\omega t_0) - 2\omega \sqrt{t_0 t} Y_1(\omega t_0) \right) J_0(\omega t) - \frac{\pi}{4} \left( \sqrt{\frac{t}{t_0}} J_0(\omega t_0) - 2\omega \sqrt{t_0 t} J_1(\omega t_0) \right) Y_0(\omega t), \\
s(t, t_0) &= -\frac{\pi}{2} \sqrt{t_0 t} Y_0(\omega t_0) J_0(\omega t) + \frac{\pi}{2} \sqrt{t_0 t} J_0(\omega t_0) Y_0(\omega t).
\end{aligned} \tag{51}$$

Note that the squared frequency is a sum of a positive constant  $\omega^2$  plus a decreasing function of time, so that the system approaches a time-independent oscillator as  $t$  tends to infinity. In Fig. 1, we show states  $\Phi_{\rho}^{(z)}(t, t_0)$  that behave as coherent states for large values of the time parameter. The classical equation of motion has a singularity at  $t = 0$  which translates into the vanishing of the uncertainty of the position operator—and, hence, into the divergence of the variance for the conjugate momentum—at that instant of time.

There are other interesting effects due to the classical singularity. Let us consider again the study of transition amplitudes developed in Section 3.4 and take  $\omega_1 = \omega_2 = \omega$ . We proceed to analyze the behavior of the (unique) state  $\Psi(t_2, t_1)$  that evolves to the vacuum state  $\Phi_0^\omega$  at time  $t_2$  when used as Cauchy data in  $t_1 < t_2$ , i.e.,

$$U(t_2, t_1) \Psi(t_2, t_1) = \Phi_0^\omega \iff \Psi(t_2, t_1) = U(t_1, t_2) \Phi_0^\omega.$$

The transition amplitudes  $\langle \Phi_{2n}^\omega | \Psi(t_2, t_1) \rangle = \langle \Phi_{2n}^\omega | U(t_1, t_2) \Phi_0^\omega \rangle$ ,  $n \in \mathbb{N}_0$ , can be computed by using Eq. (39). We recognize two regions of interest in the time domain,

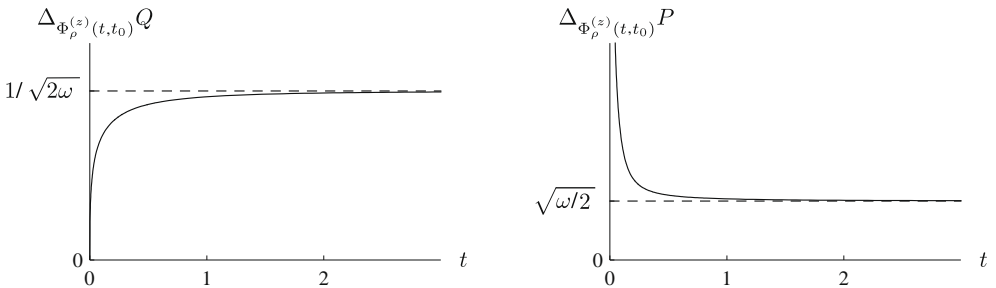
$$T_{0+} := \{(t_1, t_2) \mid 0 < t_1 \ll \omega^{-1} \ll t_2\} \quad \text{and} \quad T_{++} := \{(t_1, t_2) \mid \omega^{-1} \ll t_1 < t_2\}.$$

In  $T_{++}$ , the asymptotic behavior of the Bessel functions for large values of the time parameter [43] leads the system to behave as a TIHO of constant frequency  $\omega$ , with  $\Psi(t_2, t_1) \sim \Phi_0^\omega$ . On the other hand, in the region  $T_{0+}$ , the closeness of  $t_1$  to the classical singularity manifests itself in the form  $\Psi(t_2, t_1) \sim 0$ . Note that this behavior is in conflict with the unitary evolution of the system, which implies  $\|\Psi(t_2, t_1)\| = 1$ .

**Example 3.** ( $\mathbb{S}^1 \times \mathbb{S}^2$  and  $\mathbb{S}^3$  Gowdy-like oscillators). Gowdy models admit spatial topologies different from the 3-torus one, concretely the 3-handle  $\mathbb{S}^1 \times \mathbb{S}^2$  and the 3-sphere  $\mathbb{S}^3$ . As expected for closed universes, these systems present both initial and final singularities. For this reason, they become useful test beds to discuss the exact quantization of cyclic universes. Here, the modes satisfy equations of motion of the form

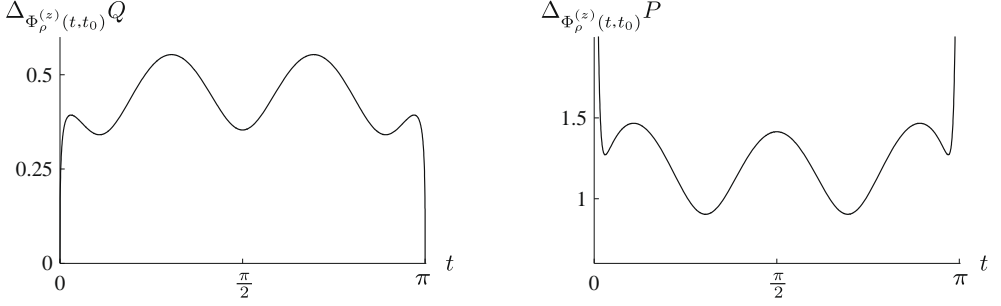
$$\ddot{u}(t) + \kappa(t; \omega) u(t) = 0, \quad \kappa(t; \omega) := \omega^2 + \frac{1}{4}(1 + \csc^2 t), \quad \omega \in \mathbb{R}, \quad t \in (0, \pi).$$

In this case, in terms of first and second class Legendre functions [43] denoted respectively as  $\mathcal{P}_x$  and  $\mathcal{Q}_x$ ,  $x \in \mathbb{R}$ , we have



**Fig. 1.** Variances of the position and momentum operators for the 3-torus Gowdy-type oscillator. Here,  $\rho(t) = \sqrt{\pi t (J_0^2(\omega t) + Y_0^2(\omega t))} / 2$ . The  $\Phi_{\rho}^{(z)}(t, t_0)$  are states of minimum uncertainty for times  $t$  far from the singularity at  $t = 0$ .





**Fig. 2.** Variances of the position and momentum operators for the 3-handle and 3-sphere Gowdy-type oscillators. Here, we take the solution  $\rho(t) = \sqrt{\sin t} \left( \mathcal{P}_{(\omega'-1)/2}^2(\cos t) + \mathcal{Q}_{(\omega'-1)/2}^2(\cos t) \right)^{1/2}$  to the auxiliary Ermakov–Pinney equation. In particular, these graphics correspond to  $\omega' = 5$ .

$$\begin{aligned}
c(t, t_0) &= \frac{1}{2} \sqrt{\sin t / \sin t_0} \mathcal{Q}_{(\omega'-1)/2}(\cos t) \left( (1 + \omega') \mathcal{P}_{(1+\omega')/2}(\cos t_0) - \omega' \mathcal{P}_{(\omega'-1)/2}(\cos t_0) \right) \\
&\quad - \frac{1}{2} \sqrt{\sin t / \sin t_0} \mathcal{P}_{(\omega'-1)/2}(\cos t) \left( (1 + \omega') \mathcal{Q}_{(1+\omega')/2}(\cos t_0) - \omega' \mathcal{Q}_{(\omega'-1)/2}(\cos t_0) \right), \\
s(t, t_0) &= \sqrt{\sin t \sin t_0} \left( \mathcal{Q}_{(\omega'-1)/2}(\cos t_0) \mathcal{P}_{(\omega'-1)/2}(\cos t) - \mathcal{P}_{(\omega'-1)/2}(\cos t_0) \mathcal{Q}_{(\omega'-1)/2}(\cos t) \right),
\end{aligned} \tag{52}$$

where  $\omega' := \sqrt{1 + 4\omega^2}$ . In Fig. 2, we show the behavior of states  $\Phi_\rho^{(z)}(t, t_0)$  for which the uncertainties of the position and momentum operators have an oscillatory behavior far enough from the singularities occurring at  $t = 0$  and  $t = \pi$ . Although  $\rho$  does not vary periodically, the function remains bounded and, thus, the  $\Phi_\rho^{(z)}(t, t_0)$  states can be used to perform a semiclassical study of these models. Finally, one may proceed as in the 3-torus case in order to analyze the way the classical singularities affect the quantum behavior of the systems, obtaining similar results.

## 5. Extension to field theories

### 5.1. General framework

In this section, we will extend the previous study to linear dynamical systems with infinite degrees of freedom, focusing our attention on the study of scalar fields evolving in fixed backgrounds such as the Minkowskian space or the so-called (linearly polarized) Gowdy metrics [24], that correspond to symmetry reductions of general relativity describing cosmological models with initial and final singularities.<sup>2</sup> Our results, however, will have a wide range of applicability, being possible to easily extend them to other field theories with similar structure. The construction of the appropriate  $C^*$ -algebra of quantum observables can be obtained by making a simple comparison with the one-dimensional case discussed in Section 3. Consider the canonical phase space  $(\Gamma, \omega)$  consisting of the infinite-dimensional  $\mathbb{R}$ -vector space  $\Gamma$  of smooth Cauchy data endowed with the natural (weakly) symplectic structure  $\omega$ . Taking the linearity of  $\Gamma$  into account, each element  $\lambda \in \Gamma$  is identified with the functional  $F_\lambda : \Gamma \rightarrow \mathbb{R}$  such that, for any other  $\lambda' \in \Gamma$ ,  $F_\lambda(\lambda') := \omega(\lambda, \lambda')$ . The abstract quantum algebra of observables is then given by the Weyl  $C^*$ -algebra on  $\Gamma$ ,  $\mathcal{W}(\Gamma)$ , generated by the elements  $W(\lambda) = \exp(iF_\lambda)$ ,  $\lambda \in \Gamma$ , that formally satisfy the relations (15). The GNS construction [12] establishes that, given any state  $\omega_0 : \mathcal{W}(\Gamma) \rightarrow \mathbb{C}$  on the algebra—that is, a normalized positive linear functional—there exist a Hilbert space  $(\mathcal{H}_0, \langle \cdot | \cdot \rangle_{\mathcal{H}_0})$ , a represen-

<sup>2</sup> The isometry group of the Gowdy models is  $U(1) \times U(1)$  and the spatial slices are restricted to have the topology of a 3-torus  $\mathbb{T}^3$ , a 3-handle  $\mathbb{S}^1 \times \mathbb{S}^2$ , a 3-sphere  $\mathbb{S}^3$ , or the lens spaces  $L(p, q)$  (that can be studied by imposing discrete symmetries on the 3-sphere case). The exact quantization of the linearly polarized Gowdy models in the vacuum or coupled to massless scalar fields has been profusely analyzed (see [25] and [27] and references therein).

tation  $\pi_0 : \mathcal{W}(\Gamma) \rightarrow \mathcal{B}(\mathcal{H}_0)$  from the Weyl algebra to the collection of bounded linear operators on  $\mathcal{H}_0$ , and a cyclic vector  $\Psi_0 \in \mathcal{H}_0$  such that

$$\omega_0(A) = \langle \Psi_0 | \pi_0(A) \Psi_0 \rangle_{\mathcal{H}_0}, \quad \forall A \in \mathcal{W}(\Gamma).$$

Moreover, the triplet  $(\mathcal{H}_0, \pi_0, \Psi_0)$  satisfying these properties is unique up to unitary equivalence. Von Neumann's uniqueness theorem, however, cannot be generalized to field theories, and states on the Weyl algebra generally yield nonequivalent cyclic representations. In order to pick out a preferred representation of the canonical commutation relations one can impose additional criterions, such as the well-known Poincaré invariance of the Fock representation for scalar fields in Minkowskian space. Regarding the Gowdy models, one imposes the invariance under an extra  $U(1)$  symmetry generated by a residual global constraint for the 3-torus case [44], or the invariance under the symmetry group  $SO(3)$  of the Klein–Gordon equations of motion for the 3-handle and the 3-sphere cases [27].

Every linear symplectic transformation  $\mathcal{T} \in \text{SP}(\Gamma)$ , for which  $\omega(\mathcal{T}\lambda_1, \mathcal{T}\lambda_2) = \omega(\lambda_1, \lambda_2)$ ,  $\lambda_1, \lambda_2 \in \Gamma$ , defines a unique  $*$ -automorphism  $\alpha_{\mathcal{T}} \in \text{Aut}(\mathcal{W}(\Gamma))$  such that  $(\alpha_{\mathcal{T}} \circ W)(\lambda) := W(\mathcal{T}\lambda)$ . This is the case, in particular, of the symplectic transformations that characterize the classical dynamics of the system. Given a concrete Hilbert space representation  $(\mathcal{H}_0, \pi_0, \Psi_0)$  of the Weyl  $C^*$ -algebra, the symplectic transformation  $\mathcal{T} \in \text{SP}(\Gamma)$  is said to be *unitarily implementable* on the cyclic representation space  $\mathcal{H}_0$  if  $\pi_0$  and  $\pi_0 \circ \alpha_{\mathcal{T}}$  are unitarily equivalent, i.e., there exists a unitary operator  $U_{\mathcal{T}} : \mathcal{H}_0 \rightarrow \mathcal{H}_0$  such that

$$U_{\mathcal{T}}^{-1} \pi(W(\lambda)) U_{\mathcal{T}} = \pi((\alpha_{\mathcal{T}} \circ W)(\lambda)), \quad \forall W(\lambda) \in \mathcal{W}(\Gamma). \quad (53)$$

A common feature of the quantization of infinite-dimensional linear symplectic dynamical systems is, precisely, the impossibility of defining the unitary quantum counterpart of *all* linear symplectic transformations on the phase space [45]. This is the case of the time evolution of the Gowdy models when these systems are written in terms of the dynamical variables that naturally appear after performing their Hamiltonian formalisms. Note, however, that the lack of a unitary operator implementing the quantum time evolution conflicts with the axiomatic structure of quantum theory itself. In case of not rejecting the models for this reason, one must analyze carefully the viability of a suitable probabilistic interpretation for them, as discussed in [46]. Nevertheless, it is possible to overcome this problem by performing some suitable time-dependent redefinitions of the basic fields [25,27]. In what follows, we will always refer to these rescaled fields.

## 5.2. Unitary quantum time evolution

The canonical phase space description of the classical systems under consideration consists now of an infinite-dimensional nonautonomous Hamiltonian system  $(I \times \Gamma, dt, \omega, H(t))$ . Here,  $\Gamma := \mathcal{C} \times \mathcal{C}$  is the space of Cauchy data, where  $\mathcal{C}$  denotes the Fréchet space of rapidly decreasing real sequences  $\mathbf{x} := (x_\ell : \ell \in \mathbb{X})$ , with  $\ell$  running over some countable set  $\mathbb{X}$  [47–49]. This space is endowed with the natural symplectic structure

$$\omega((\mathbf{q}_1, \mathbf{p}_1), (\mathbf{q}_2, \mathbf{p}_2)) := \sum_{\ell \in \mathbb{X}} (p_{1\ell} q_{2\ell} - p_{2\ell} q_{1\ell}), \quad \forall (\mathbf{q}_1, \mathbf{p}_1), (\mathbf{q}_2, \mathbf{p}_2) \in \Gamma.$$

The time-dependent Hamiltonian  $H(t) : \Gamma \rightarrow \mathbb{R}$  is a quadratic form on  $\Gamma$  that can be diagonalized as a sum of TDHO Hamiltonians of the type (13). Explicitly,

$$H(t, \mathbf{q}, \mathbf{p}) := \frac{1}{2} \sum_{\ell \in \mathbb{X}} (p_\ell^2 + \kappa_\ell(t) q_\ell^2), \quad t \in I = (t_-, t_+) \subseteq \mathbb{R}, \quad (54)$$

where the time-dependent squared frequencies  $\kappa_\ell(t) \in C^0(I)$ ,  $\ell \in \mathbb{X}$ , must satisfy  $\boldsymbol{\kappa}(t) = (\kappa_\ell(t) : \ell \in \mathbb{X}) \in \bar{\mathcal{C}}$ , for all  $t \in I$ , with  $\bar{\mathcal{C}}$  denoting the vector space of slowly increasing real sequences, i.e., the topological dual of  $\mathcal{C}$ . The time evolution is implemented by symplectic transformations of the type (14)

$$\begin{pmatrix} q_{tH}(t, t_0) \\ p_{tH}(t, t_0) \end{pmatrix} = T_{(t, t_0)}^{(\ell)} \cdot \begin{pmatrix} q_\ell \\ p_\ell \end{pmatrix}, \quad T_{(t, t_0)}^{(\ell)} := \begin{pmatrix} c_\ell(t, t_0) & s_\ell(t, t_0) \\ \dot{c}_\ell(t, t_0) & \dot{s}_\ell(t, t_0) \end{pmatrix}, \quad \ell \in \mathbb{X},$$

where, for each  $\ell \in \mathbb{X}$ ,  $c_\ell$  and  $s_\ell$  are the solutions to the TDHO equation of squared frequency  $\kappa_\ell(t)$  introduced in Section 2.

For the Minkowskian quantum field theory generalized to a spacetime  $\mathbb{R} \times \mathbb{T}^3$  with closed spatial sections we have  $\mathbb{X} = \mathbb{Z} \setminus \{0\}$  and  $\kappa_\ell(t) = |\ell|^2$ , for all  $t \in \mathbb{R}$ . For the 3-torus Gowdy models [25] we take  $\mathbb{X} = \mathbb{Z} \setminus \{0\}$  and  $\kappa_\ell(t) = |\ell|^2 + 1/(4t^2)$ , with  $t \in (0, +\infty)$ . For the remaining topologies admitted by the Gowdy cosmologies, the 3-handle and the 3-sphere [27],  $\mathbb{X} = \mathbb{N}$  and  $\kappa_\ell(t) = \ell(\ell + 1) + (1 + \csc^2 t)/4$ , with  $t \in (0, \pi)$ . For simplicity, we will not consider in these cases the quantization of the zero mode  $\ell = 0$ . It can be represented in terms of standard position and momentum operators with dense domains in  $L^2(\mathbb{R})$ . The  $c_\ell$  and  $s_\ell$  functions for the Minkowskian and Gowdy 3-torus cases are respectively given by (3) and (51) substituting  $\omega = |\ell|$ ; for the 3-handle and 3-sphere topologies, they are given by (52) identifying  $\omega = \sqrt{\ell(\ell + 1)}$ . The classical singularities of the Gowdy models will persist in their quantum formulations.

In order to exactly quantize the infinite-dimensional systems under consideration, we introduce Schrödinger representations [50–53], where state vectors act as functionals  $\Psi : \bar{\mathcal{C}} \rightarrow \mathbb{C}$  belonging to certain Hilbert spaces  $\mathcal{H}_\alpha = L^2(\bar{\mathcal{C}}, \sigma(\text{Cyl}(\bar{\mathcal{C}})), d\mu_\alpha)$ , and define suitable decompositions of the position and momentum operators in terms of modes. There are subtleties associated with the infinite-dimensionality of the classical configuration space  $\mathcal{C}$  that affect the definition of the Hilbert space. On one hand, it is not possible to define nontrivial Lebesgue-type translation invariant measures  $\mu_\alpha$ , but rather probability ones [49, 54]. On other hand, set over which the measure space is built—the so-called quantum configuration space—must be given by some suitable distributional extension of  $\mathcal{C}$ . In this case, it suffices to consider the dual  $\bar{\mathcal{C}}$ . The reason to proceed in this way is that the measure is not supported on  $\mathcal{C}$ , i.e., the classical configuration space has zero measure with respect to  $\mu_\alpha$ . Given a nonzero complex sequence  $\alpha = (\alpha_\ell : \ell \in \mathbb{X})$ , the Gaussian measure  $\mu_\alpha$  is defined on the cylinder sets  $\sigma$ -algebra  $\sigma(\text{Cyl}(\bar{\mathcal{C}}))$  on  $\bar{\mathcal{C}}$ . This is the smallest  $\sigma$ -algebra with respect to which the functionals  $\mathbf{q} \in \bar{\mathcal{C}} \mapsto \langle \mathbf{q}, \mathbf{x} \rangle := \sum_{\ell \in \mathbb{X}} q_\ell x_\ell$  are measurable for each  $\mathbf{x} \in \mathcal{C}$ . Explicitly, for each finite  $n$ -tuple  $(\ell_1, \dots, \ell_n) \in \mathbb{X}^n$ , such that  $\ell_i < \ell_{i+1}$  ( $i = 1, \dots, n-1$ ), let us consider the projections  $p_{\ell_1 \dots \ell_n} : \bar{\mathcal{C}} \rightarrow \mathbb{R}^n$ ,  $\mathbf{q} \mapsto p_{\ell_1 \dots \ell_n}(\mathbf{q}) = (q_{\ell_1}, \dots, q_{\ell_n})$ . Then,  $\mu_\alpha$  is defined by its action on cylinder sets belonging to  $\sigma$ -algebras of the form  $\mathcal{B}_{\ell_1 \dots \ell_n}(\bar{\mathcal{C}}) = p_{\ell_1 \dots \ell_n}^{-1}(\mathcal{B}(\mathbb{R}^n)) \subset \sigma(\text{Cyl}(\bar{\mathcal{C}}))$ , where  $\mathcal{B}(\mathbb{R}^n)$  is the Borel  $\sigma$ -algebra of subsets of  $\mathbb{R}^n$ , i.e.,

$$d\mu_\alpha|_{\mathcal{B}_{\ell_1 \dots \ell_n}} = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}|\alpha_{\ell_i}|} \exp \left( -\frac{q_{\ell_i}^2}{2|\alpha_{\ell_i}|^2} \right) dq_{\ell_i}.$$

The sequence  $\alpha$  defines a positive continuous nondegenerate bilinear form  $C_\alpha : \mathcal{C} \times \mathcal{C} \rightarrow \mathbb{R}$  through the formula  $C_\alpha(\mathbf{x}, \mathbf{y}) := \sum_{\ell \in \mathbb{X}} |\alpha_\ell|^2 x_\ell y_\ell$ ,  $\mathbf{x}, \mathbf{y} \in \mathcal{C}$ .  $C_\alpha$  is called the *covariance* operator in this context [48].

We consider now certain class of measurable functions that we will use in the following. Let  $\mathcal{X} \subset \mathcal{C}$  be a finite dimensional subspace of the classical configuration space  $\mathcal{C}$ . A cylinder function  $\Psi$ , based on  $\mathcal{X}$ , is a function of the form

$$\Psi(\mathbf{q}) = F(\langle \mathbf{q}, \mathbf{x}_1 \rangle, \dots, \langle \mathbf{q}, \mathbf{x}_n \rangle)$$

for a finite set  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathcal{X}$ , where  $F : \mathbb{R}^n \rightarrow \mathbb{C}$  is a smooth function. They are called cylinder because they depend on  $\mathbf{q} \in \bar{\mathcal{C}}$  through the pairings  $\langle \mathbf{q}, \mathbf{x}_i \rangle$  defined by a finite number of “probes”  $\mathbf{x}_i \in \mathcal{C}$ . The Gaussian measure  $\mu_\alpha$  can be used to endow the linear space spanned by this type of functions with an inner product. Explicitly, in the particular case  $\mathcal{X} = \text{span}\{\mathbf{e}_{\ell_1}, \dots, \mathbf{e}_{\ell_n}\}$ , where  $\mathbf{e}_\ell \in \mathcal{C}$  denotes a sequence whose only nonzero component is the  $\ell$ th one, every cylinder function  $\Psi$  on  $\mathcal{X}$  can be written in the form  $\Psi(\mathbf{q}) = F(q_{\ell_1}, \dots, q_{\ell_n})$  and the scalar product is given by

$$\langle \Psi_1 | \Psi_2 \rangle = \int_{\mathbb{R}^n} \bar{F}_1(q_{\ell_1}, \dots, q_{\ell_n}) F_2(q_{\ell_1}, \dots, q_{\ell_n}) \prod_{i=1}^n \frac{1}{\sqrt{2\pi}|\alpha_{\ell_i}|} \exp \left( -\frac{q_{\ell_i}^2}{2|\alpha_{\ell_i}|^2} \right) dq_{\ell_i}.$$

Square integrable cylinder functions on  $\mathcal{X}$  span a  $\mathbb{C}$ -vector space that we denote as  $\text{Cyl}_{\mathcal{X}}$ . The class of all cylinder functions is denoted by  $\text{Cyl} := \cup_{\mathcal{X}} \text{Cyl}_{\mathcal{X}}$ . The inner products defined on each  $\text{Cyl}_{\mathcal{X}}$  can be extended to  $\text{Cyl}$  in the natural way and the Cauchy completion of  $\text{Cyl}$  with respect to this inner product is the Hilbert space  $\mathcal{H}_{\mathbf{x}}$  (see [54] for more details).

The configuration observables will act as multiplication operators, whereas the canonically conjugate momenta will differ from the usual ones in terms of derivatives by the appearance of multiplicative terms which are necessary to ensure their self-adjointness; specifically, for  $\Psi \in \text{Cyl}$ ,

$$(Q_{\ell}\Psi)(\mathbf{q}) = q_{\ell}\Psi(\mathbf{q}), \quad (P_{\ell}\Psi)(\mathbf{q}) = -i\frac{\partial\Psi}{\partial q_{\ell}}(\mathbf{q}) + \frac{\bar{\beta}_{\ell}}{\alpha_{\ell}}q_{\ell}\Psi(\mathbf{q}). \quad (55)$$

The complex sequences  $\alpha$  and  $\beta$  must satisfy

$$\alpha_{\ell}\bar{\beta}_{\ell} - \beta_{\ell}\bar{\alpha}_{\ell} = i, \quad \forall \ell \in \mathbb{X}, \quad (56)$$

by virtue of the CCR,  $[Q_{\ell}, P_{\ell'}] = i\delta(\ell, \ell')\mathbf{1}$  and  $[Q_{\ell}, Q_{\ell'}] = 0 = [P_{\ell}, P_{\ell'}]$ . These conditions imply  $|\alpha_{\ell}||\beta_{\ell}| \geq 1/2$  for all  $\ell \in \mathbb{X}$ . The functional form of  $\alpha$  and  $\beta$  for the Minkowskian case and Gowdy models will be discussed later in the context of the unitary implementability of their dynamics.

According to condition (53), if the quantum dynamics is unitarily implementable there exists a (biparametric) family of unitary operators  $U(t, t_0) : \mathcal{H}_{\mathbf{x}} \rightarrow \mathcal{H}_{\mathbf{x}}$ , depending on  $(t, t_0) \in I \times I$ , such that

$$U^{-1}(t, t_0)Q_{\ell}U(t, t_0) = c_{\ell}(t, t_0)Q_{\ell} + s_{\ell}(t, t_0)P_{\ell}, \quad (57)$$

$$U^{-1}(t, t_0)P_{\ell}U(t, t_0) = \dot{c}_{\ell}(t, t_0)Q_{\ell} + \dot{s}_{\ell}(t, t_0)P_{\ell}. \quad (58)$$

The above relations characterize  $U(t, t_0)$  univocally up to phase. They can be rewritten in terms of annihilation and creation operators  $a_{\ell}$  and  $a_{\ell}^*$ , with  $[a_{\ell}, a_{\ell'}^*] = \delta(\ell, \ell')\mathbf{1}$  and  $[a_{\ell}, a_{\ell'}] = 0 = [a_{\ell}^*, a_{\ell'}^*]$ , such that

$$Q_{\ell} = \alpha_{\ell}a_{\ell} + \bar{\alpha}_{\ell}a_{\ell}^*, \quad P_{\ell} = \beta_{\ell}a_{\ell} + \bar{\beta}_{\ell}a_{\ell}^* \iff a_{\ell} = -i\bar{\beta}_{\ell}Q_{\ell} + i\bar{\alpha}_{\ell}P_{\ell}, \quad a_{\ell}^* = i\beta_{\ell}Q_{\ell} - i\alpha_{\ell}P_{\ell}. \quad (59)$$

Relations (57) and (58) are then equivalent to

$$U^{-1}(t, t_0)a_{\ell}U(t, t_0) = A_{\ell}(t, t_0)a_{\ell} + B_{\ell}(t, t_0)a_{\ell}^*, \quad (60)$$

$$U^{-1}(t, t_0)a_{\ell}^*U(t, t_0) = \bar{B}_{\ell}(t, t_0)a_{\ell} + \bar{A}_{\ell}(t, t_0)a_{\ell}^*,$$

where the Bogoliubov coefficients  $A_{\ell}(t, t_0)$  and  $B_{\ell}(t, t_0)$  are given by

$$A_{\ell}(t, t_0) := i(\dot{s}_{\ell}(t, t_0)\bar{\alpha}_{\ell}\beta_{\ell} - c_{\ell}(t, t_0)\bar{\beta}_{\ell}\alpha_{\ell} + \dot{c}_{\ell}(t, t_0)|\alpha_{\ell}|^2 - s_{\ell}(t, t_0)|\beta_{\ell}|^2), \quad (61)$$

$$B_{\ell}(t, t_0) := i(\dot{s}_{\ell}(t, t_0) - c_{\ell}(t, t_0))\bar{\alpha}_{\ell}\bar{\beta}_{\ell} + \dot{c}_{\ell}(t, t_0)\bar{\alpha}_{\ell}^2 - s_{\ell}(t, t_0)\bar{\beta}_{\ell}^2, \quad (62)$$

satisfying  $|A_{\ell}(t, t_0)|^2 - |B_{\ell}(t, t_0)|^2 = 1$ , for all  $\ell \in \mathbb{X}$ . In particular,  $A_{\ell}(t, t_0) \neq 0$  for all  $(t, t_0) \in I \times I$ . According to the theory of unitary implementation of symplectic transformations [45], the unitary time evolution operator  $U(t, t_0)$  exists if and only if

$$\mathbf{B}(t, t_0) = (B_{\ell}(t, t_0) : \ell \in \mathbb{X}) \in \ell^2(\mathbb{C}) \iff \sum_{\ell \in \mathbb{X}} |B_{\ell}(t, t_0)|^2 < +\infty, \quad \forall (t, t_0) \in I \times I. \quad (63)$$

For quantum free fields in Minkowskian spacetime the usual choice

$$\alpha_{\ell} = \frac{1}{\sqrt{2|\ell|}} \quad \text{and} \quad \beta_{\ell} = -i\sqrt{\frac{|\ell|}{2}} \quad (64)$$

implies  $\mathbf{B}(t, t_0) = \mathbf{0}$  and, as is well known, the time evolution is unitarily implementable for inertial observers. The uniqueness of this representation can be proved by using the same techniques employed in the standard  $\mathbb{R} \times \mathbb{R}^3$  Minkowskian spacetime under the condition of Poincaré invariance. Concerning the Gowdy models, it is straightforward to show that the unitarity of the quantum time evolution is guaranteed for  $\alpha$  and  $\beta$  sequences with the asymptotic expansions (see [25–27] for more details)

$$\alpha_{\ell} = \frac{1}{\sqrt{2|\ell|}} \exp(i\gamma_{\ell}) + O(|\ell|^{-3/2}), \quad \beta_{\ell} = -i\sqrt{\frac{|\ell|}{2}} \exp(i\gamma_{\ell}) + O(|\ell|^{-1/2}),$$

where  $\gamma$  is an arbitrary real-valued sequence. Moreover, all ( $U(1)$  or  $SO(3)$ -invariant) representations for which the dynamics is well-defined and unitary are unitarily equivalent. In what follows, we will assume the use of the particular choice of  $\alpha$  and  $\beta$  coincident with Eq. (64). As a counterexample to the previous cases with unitary evolution, consider a system of infinitely many harmonic oscillators with imaginary frequency of the type (5). In this case, it is possible to show the nonexistence of sequences  $\alpha$  and  $\beta$  satisfying (56) such that the dynamics is unitarily implemented. The ‘wrong sign’ of the squared frequency is also responsible for the failure of the unitarity of the time evolution in more complicated systems, such as minimally coupled massless scalar fields evolving in de Sitter spacetime [55].

Note that the annihilation operators are given by the derivatives

$$a_\ell = \bar{\alpha}_\ell \frac{\partial}{\partial q_\ell}$$

and, hence, the vacuum state  $\Psi_0 \in \mathcal{H}_\alpha$  satisfying  $a_\ell \Psi_0 = 0$  for all  $\ell \in \mathbb{X}$  is given by the unit constant functional  $\Psi_0(\mathbf{q}) = 1$  up to multiplicative phase. The states with finite number of particles, which are obtained as the image of any polynomial in the creation operators acting on the vacuum state, define a common, invariant, dense domain of analytic vectors for the configuration and momentum operators (55), so that their essential self-adjointness is guaranteed and, hence, the existence of unique self-adjoint extensions (see Nelson’s analytic vector theorem in [56]).

From the Bogoliubov transformations (60), and proceeding as in the one-dimensional case (44), one easily computes the evolution of the vacuum state,

$$U(t, t_0) \Psi_0 = \langle \Psi_0 | U(t, t_0) \Psi_0 \rangle \exp \left( -\frac{1}{2} \sum_{\ell \in \mathbb{X}} \frac{B_\ell(t_0, t)}{A_\ell(t_0, t)} a_\ell^2 \right) \Psi_0, \quad (65)$$

with

$$|\langle \Psi_0 | U(t, t_0) \Psi_0 \rangle| = \prod_{\ell \in \mathbb{X}} \frac{1}{\sqrt{|A_\ell(t_0, t)|}}. \quad (66)$$

Due to the unitary implementability of the dynamics, the square summability of the sequence  $(B_\ell(t_0, t)/A_\ell(t_0, t) : \ell \in \mathbb{X})$  and the convergence of  $\sum_{\ell \in \mathbb{X}} \log |A_\ell(t_0, t)|$  are guaranteed and, hence, the action of  $U(t, t_0)$  is well defined over states with finite number of particles. The phase of the expectation value (66), though being irrelevant to answer most of the physical questions, can be explicitly calculated once a quantum Hamiltonian has been fixed. The Hamiltonian verifies Eq. (20) and coincides with the operator directly promoted from the classical expression (54) modulo an arbitrary  $t$ -dependent real term proportional to the identity which encodes the choice of  $U(t, t_0)$ , i.e.,

$$H(t) = \frac{1}{2} \sum_{\ell \in \mathbb{X}} \left( P_\ell^2 + \kappa_\ell(t) Q_\ell^2 + 2\vartheta_\ell(t) \mathbf{1} \right),$$

where the sequence  $\vartheta_\ell(t) \in C^0(I)$ ,  $\ell \in \mathbb{X}$ , is usually employed to avoid the appearance of infinite phases. Analogously to the one-dimensional case, when the dynamics is unitarily implementable, we define the time evolution propagator through the relation

$$(U(t, t_0) \Psi)(\mathbf{q}) = \int_{\mathbb{C}} K_{\alpha\beta}(\mathbf{q}, t; \mathbf{q}_0, t_0) \Psi(\mathbf{q}_0) d\mu_\alpha(\mathbf{q}_0),$$

where a straightforward calculation formally provides

$$K_{\alpha\beta}(\mathbf{q}, t; \mathbf{q}_0, t_0) = \prod_{\ell \in \mathbb{X}} \sqrt{2\pi} |\alpha_\ell| \exp \left( \frac{i}{2} \left( \frac{\beta_\ell}{\alpha_\ell} q_{0\ell}^2 - \frac{\bar{\beta}_\ell}{\bar{\alpha}_\ell} q_\ell^2 \right) \right) K_\ell(q_\ell, t; q_{0\ell}, t_0) \exp \left( -i \int_{t_0}^t d\tau \vartheta_\ell(\tau) \right), \quad (67)$$

with  $K_\ell$  denoting the propagator (22) associated with the one-dimensional oscillator of squared frequency  $\kappa_\ell(t)$ . The reader may wish to compare this expression with Eq. (25) corresponding to a single oscillator. This formula coincides with the one obtained in [57] when restricted to generic finite

dimensional and time-dependent linear Hamiltonian systems. For the sequences (64), Eq. (67) provides the expectation value

$$\langle \Psi_0 | U(t, t_0) \Psi_0 \rangle = \prod_{\ell \in \mathbb{X}} \frac{1}{\sqrt{|A_\ell(t_0, t)|}} \exp \left( i \left( \sigma_\ell(t, t_0) - \int_{t_0}^t d\tau \vartheta_\ell(\tau) \right) \right),$$

with

$$\sigma_\ell(t, t_0) = -\frac{1}{2} \arctan \frac{|\ell| s_\ell(t, t_0) - |\ell|^{-1} \dot{c}_\ell(t, t_0)}{c_\ell(t, t_0) + \dot{s}_\ell(t, t_0)}$$

for times  $t$  close to  $t_0$ . For the Minkowskian free fields, as in the one-dimensional case, the phases  $\sigma_\ell(t, t_0)$  can be exactly canceled for all  $\ell \in \mathbb{Z} \setminus \{0\}$  just by defining a normal ordered quantum Hamiltonian, which amounts to choosing  $\vartheta_\ell(t) = -|\ell|/2$ . In general, however, it is not possible to eliminate them. For the Gowdy cosmologies, attending to the fact that the  $c_\ell$  and  $s_\ell$  functions tend to those corresponding to the Minkowskian case for large values of  $|\ell|$ , it is easy to check that normal ordering allows only the cancelation of the phases at high frequencies, with  $\vartheta_\ell(t) \sim -|\ell|/2$  as  $|\ell| \rightarrow +\infty$ .

Since we are dealing with systems of infinite number of uncoupled oscillators, one would expect that the analysis developed in Section 3 for a single oscillator would allow us to factorize the evolution operator in the form

$$U(t, t_0) = T_\rho^{-1}(t) R_\rho(t, t_0) T_\rho(t_0), \quad (68)$$

where, given a sequence  $\rho(t) = (\rho_\ell(t) : \ell \in \mathbb{X})$  of solutions to the auxiliary Ermakov–Pinney equations  $\ddot{\rho}_\ell + \kappa_\ell(t) \rho_\ell = 1/\rho_\ell^3$ , the  $T_\rho(t)$  and  $R_\rho(t, t_0)$  operators are univocally characterized up to phases by their action on annihilation and creation operators,

$$\begin{aligned} T_\rho^{-1}(t) a_\ell T_\rho(t) &= i \left( \beta_\ell \bar{\alpha}_\ell \rho_\ell(t) - \frac{\alpha_\ell \bar{\beta}_\ell}{\rho_\ell(t)} - |\alpha_\ell|^2 \dot{\rho}_\ell(t) \right) a_\ell + i \left( \bar{\alpha}_\ell \bar{\beta}_\ell \left( \rho_\ell(t) - \frac{1}{\rho_\ell(t)} \right) - \bar{\alpha}_\ell^2 \dot{\rho}_\ell(t) \right) a_\ell^*, \\ R_\rho^{-1}(t, t_0) a_\ell R_\rho(t, t_0) &= \left( \cos \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) - i(|\alpha_\ell|^2 + |\beta_\ell|^2) \sin \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) \right) a_\ell - i(\bar{\alpha}_\ell^2 + \bar{\beta}_\ell^2) \sin \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) a_\ell^*, \end{aligned}$$

and similarly for  $a_\ell^*$ . Again, the resulting unitary evolution operator should be independent of the particular choice of  $\rho$  since, as we have shown above, the propagator does not depend on it. However, even in the case of  $U(t, t_0)$  being well-defined as unitary operator, the factorization (68) may be ill-defined. This is, in fact, the case for free fields evolving in Minkowskian and Gowdy-type spacetimes, as we will prove below. Obviously, this does not prevent us from defining another well-defined factorizations for  $U(t, t_0)$  different from (68). A particularly convenient choice is the one made in [26] for the 3-torus Gowdy model. Calculations developed there can be translated essentially unchanged into the remaining Gowdy spatial topologies and the Minkowskian case (see the Appendix A). Here, however, we are interested in the original factorization due to its implications for the search of semiclassical states. According to [45], the necessary and sufficient condition for  $T_\rho(t)$  to be unitary for each value of  $t$  is given by

$$\sum_{\ell \in \mathbb{X}} |\alpha_\ell \beta_\ell (\rho_\ell(t) - 1/\rho_\ell(t)) - \alpha_\ell^2 \dot{\rho}_\ell(t)|^2 < +\infty, \quad \forall t \in I. \quad (69)$$

Similarly, it is straightforward to show that  $R_\rho(t, t_0)$  is unitarily implementable if and only if

$$\sum_{\ell \in \mathbb{X}} \left| (\alpha_\ell^2 + \beta_\ell^2) \sin \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) \right|^2 < +\infty, \quad \forall (t, t_0) \in I \times I. \quad (70)$$

Eq. (64) for quantum free fields in Minkowskian and Gowdy-type spacetimes lead us to conclude that conditions (69) and (70) are not satisfied and, hence, neither  $T_\rho(t)$  nor  $R_\rho(t, t_0)$  are unitary in those systems. In the case of  $R_\rho(t, t_0)$ , this conclusion follows readily, irrespective of  $\rho(t)$ . For  $T_\rho(t)$ , a necessary condition for (69) to be satisfied is given by

$$\sum_{\ell \in \mathbb{X}} |\rho_\ell(t) - 1/\rho_\ell(t)|^2 < +\infty \iff \lim_{|\ell| \rightarrow +\infty} \rho_\ell(t) = 1, \quad \forall t \in I,$$

where we have taken into account the fact that the real sequence  $(\rho_\ell(t) : \ell \in \mathbb{X})$  is positive and bounded for all  $t$ . According to Eq. (12), this implies  $s_\ell(t, t_0) \sim \sin C(t, t_0)$  as  $|\ell| \rightarrow +\infty$ , where  $C(t, t_0)$  is a *nonzero* function which depends on the system and whose form we do not need to specify. This is in conflict with the asymptotic behavior of  $s_\ell(t, t_0)$  for the systems under study, given by  $s_\ell(t, t_0) \sim 0$  as  $|\ell| \rightarrow +\infty$  for all  $(t, t_0) \in I \times I$ .

### 5.3. Semiclassical states

The explicit expression of the quantum unitary evolution for the single harmonic oscillator as a product of unitary operators (see Theorem 3 in Section 3) turned out to be very useful to construct semiclassical states for some relevant one-dimensional dynamical systems. In particular, as stated in (31), the operator  $T_\rho(t)$  transforms the Lewis invariant (30) into the time independent free Hamiltonian (29). However, as we have shown in Section 5.2, there are obstructions that arise when dealing with systems of infinite oscillators—particularly, the possible nonunitarity of  $T_\rho(t)$ —making the application of the techniques developed in Section 4 particularly difficult. In order to avoid these difficulties, we will probe an alternative procedure to construct semiclassical states that takes advantage of the unitary implementability of the quantum time evolution. We start by constructing the analogs of the minimal wave packets of the one-dimensional harmonic oscillator. Given a square summable sequence  $\mathbf{z} = (z_\ell : \ell \in \mathbb{X}) \in \ell^2(\mathbb{C})$ , consider the state

$$\Phi^{(\mathbf{z})} := e^{-\|\mathbf{z}\|^2/2} \exp \left( \sum_{\ell \in \mathbb{X}} z_\ell a_\ell^* \right) \Psi_0 \in \mathcal{H}_\mathbf{z}, \quad (71)$$

where the vacuum state  $\Psi_0$  corresponds in this context to  $\mathbf{z} = 0$ , and  $\|\mathbf{z}\| = \sum_{\ell \in \mathbb{X}} |z_\ell|^2$ . Vectors defined in this way appear as coherent superpositions of states with arbitrary number of particles. We then introduce the annihilation and creation operators in the Heisenberg picture corresponding to evolution *backwards* in time,

$$\begin{aligned} a_\ell(t, t_0) &:= U(t, t_0) a_\ell U^{-1}(t, t_0) = \bar{A}_\ell(t, t_0) a_\ell - B_\ell(t, t_0) a_\ell^*, \\ a_\ell^*(t, t_0) &:= U(t, t_0) a_\ell^* U^{-1}(t, t_0) = -\bar{B}_\ell(t, t_0) a_\ell + A_\ell(t, t_0) a_\ell^*, \end{aligned}$$

satisfying the Heisenberg algebra for all  $(t, t_0) \in I \times I$ . Here,  $A_\ell(t, t_0)$  and  $B_\ell(t, t_0)$  are the Bogoliubov coefficients defined in (61) and (62), respectively. We then evolve the states (71) in the Schrödinger picture, obtaining

$$\begin{aligned} \Phi^{(\mathbf{z})}(t, t_0) &:= U(t, t_0) \Phi^{(\mathbf{z})} = e^{-\|\mathbf{z}\|^2/2} U(t_0, t) \exp \left( \sum_{\ell \in \mathbb{X}} z_\ell a_\ell^* \right) \Psi_0 \\ &= e^{-\|\mathbf{z}\|^2/2} \exp \left( \sum_{\ell \in \mathbb{X}} z_\ell a_\ell^*(t_0, t) \right) \Phi^{(\mathbf{0})}(t, t_0), \end{aligned}$$

with  $a_\ell(t_0, t) \Phi^{(\mathbf{z})}(t, t_0) = z_\ell \Phi^{(\mathbf{z})}(t, t_0)$ ,  $\forall \ell \in \mathbb{X}$ , and  $\Phi^{(\mathbf{0})}(t, t_0) = U(t, t_0) \Psi_0$ . By definition, the one-parameter family of states obtained in this way verifies the Schrödinger equation with initial condition  $\Phi^{(\mathbf{z})}$ , and is closed under time evolution as well,  $U(t_2, t_1) \Phi^{(\mathbf{z})}(t_1, t_0) = \Phi^{(\mathbf{z})}(t_2, t_0)$ . The states  $\Phi^{(\mathbf{z})}(t, t_0)$  satisfy the properties stated in the following theorem.

**Theorem 6.** *Let  $\mathbf{z} = (z_\ell : \ell \in \mathbb{X}) \in \ell^2(\mathbb{C})$  and  $t_0 \in I$ . The position and momentum expectation values in the state  $\Phi^{(\mathbf{z})}(t, t_0) = U(t, t_0) \Phi^{(\mathbf{z})}$  satisfy*

$$\begin{aligned} q_{H_\ell}(t, t_0) &= \langle \Phi^{(\mathbf{z})}(t, t_0) | Q_\ell \Phi^{(\mathbf{z})}(t, t_0) \rangle = 2c_\ell(t, t_0) \text{Re}(\alpha_\ell z_\ell) + 2s_\ell(t, t_0) \text{Re}(\beta_\ell z_\ell), \\ p_{H_\ell}(t, t_0) &= \langle \Phi^{(\mathbf{z})}(t, t_0) | P_\ell \Phi^{(\mathbf{z})}(t, t_0) \rangle = 2\dot{c}_\ell(t, t_0) \text{Re}(\alpha_\ell z_\ell) + 2\dot{s}_\ell(t, t_0) \text{Re}(\beta_\ell z_\ell), \end{aligned}$$

where  $(q_{H\ell}, p_{H\ell})$  is the classical solution (14) determined by the Cauchy data  $(q_\ell, p_\ell) = (2\text{Re}(\alpha_\ell z_\ell), 2\text{Re}(\beta_\ell z_\ell))$  at time  $t_0$ . Moreover, the mean square deviations of the position and momentum operators with respect to the evolved state  $\Phi^{(\mathbf{z})}(t, t_0)$  satisfy

$$\Delta_{\Phi^{(\mathbf{z})}(t, t_0)} Q_\ell = |\alpha_\ell A_\ell(t, t_0) + \bar{\alpha}_\ell \bar{B}_\ell(t, t_0)|, \quad \Delta_{\Phi^{(\mathbf{z})}(t, t_0)} P_\ell = |\beta_\ell A_\ell(t, t_0) + \bar{\beta}_\ell \bar{B}_\ell(t, t_0)|,$$

irrespective of  $\mathbf{z}$ .

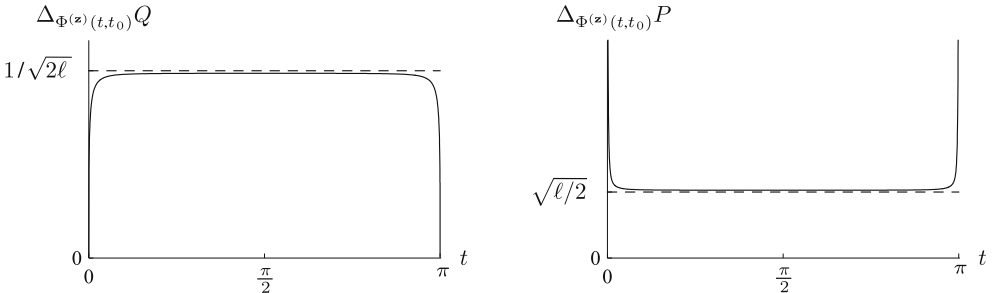
**Remark 7.** Let us consider the Gowdy models. As a consequence of the unitary implementability of the dynamics (63), we have  $\mathbf{B}(t, t_0) \in \ell^2(\mathbb{C})$  and, hence,  $|A_\ell(t, t_0)| \sim 1$  as  $|\ell| \rightarrow +\infty$ . We then obtain (see Fig. 3)

$$\Delta_{\Phi^{(\mathbf{z})}(t, t_0)} Q_\ell \sim |\alpha_\ell| = \frac{1}{\sqrt{2|\ell|}}, \quad \Delta_{\Phi^{(\mathbf{z})}(t, t_0)} P_\ell \sim |\beta_\ell| = \sqrt{\frac{|\ell|}{2}} \quad \text{when } |\ell| \rightarrow +\infty. \quad (72)$$

For fixed values of  $t_0$ , these asymptotic behaviors converge uniformly in  $t$  for time intervals away from the classical singularities. Note that these behaviors are the same that one would have expected to obtain if it had been possible to suitably extend the study developed in Section 4 to field theories. We then conclude that the  $\Phi^{(\mathbf{z})}(t, t_0)$  vectors are coherent states far enough from the singularities. For the 3-torus model, the sequence  $\mathbf{z} \in \ell^2(\mathbb{C})$  is subject to satisfy a global constraint remaining on the system, given by  $\sum_{\ell \in \mathbb{Z} \setminus \{0\}} \ell |z_\ell|^2 = 0$ . In the Minkowskian case, expressions (72) are valid for all  $\ell \in \mathbb{Z} \setminus \{0\}$ .

## 6. Conclusions

In this paper, we have revised the unitary implementability of the quantum dynamics of a time-dependent harmonic oscillator (TDHO) and used the theory of invariants in order to define suitable semiclassical states for some relevant systems, such as the vertically driven pendulum or Gowdy-like oscillators. In particular, we have analyzed some important issues related to the associated Ermakov–Pinney equation, clarifying the need to introduce it as a natural way to obtain an evolution operator valid for *all* values of the time parameter. We must emphasize again that other elections different from the auxiliary Ermakov–Pinney equation may be problematic because of the singular behavior of the resulting evolution operator. We have shown that the Feynman propagator, usually derived by making use of more complicated path-integration techniques, can be obtained in a straightforward way within this scheme. The resulting formula has then been applied to calculate transition amplitudes, the instability of the vacuum state, and semiclassical states. Most of the calculations regarding the quantum



**Fig. 3.** Asymptotic behavior of the variances of the field and momentum operators  $Q_\ell$  and  $P_\ell$  for the states  $\Phi^{(\mathbf{z})}(t, t_0)$ ,  $t_0 < t \in (0, \pi)$ , at high frequencies (limit  $\ell \rightarrow +\infty$ ) for the 3-handle and 3-sphere Gowdy models. Note the purely quantum behavior of these states as  $t$  approaches the classical singularities. These graphics can be considered as the limit of Fig. 2 for large frequencies. The asymptotic behavior for the 3-torus case is similar to the one represented in Fig. 1, identifying  $\omega = |\ell|$  for each mode.



evolution can be performed just by taking the classical dynamics into account, except for the presence of a phase that depends on the election of the quantum Hamiltonian. Nevertheless, this phase is irrelevant to answer all relevant physical questions such as the calculation of probability amplitudes or the evolution of quantum observables. It is important to remark that this phase, in contrast with the situation for the well-known TIHO system, cannot be eliminated in all cases by considering normal ordered Hamiltonians.

Although we have concentrated our discussion on the quantum TDHO, our results can be easily extended to another interesting cases. For instance, our study is also applicable to the harmonic oscillator driven by an external, nonstationary, perturbative force characterized by a linear term in the position operator,

$$H(t) = \frac{1}{2} \left( P^2 + \kappa(t) Q^2 \right) + f(t) Q, \quad f \in C^1(I).$$

Indeed, this Hamiltonian can be transformed into the Hamiltonian (21) just by introducing an  $f$ -dependent Glauber displacement operator [21,58].

Finally, we have extended the study of the unitary evolution of a single quantum harmonic oscillator to systems of infinite number of uncoupled oscillators with time-dependent frequency, concretely, to the quantum field theory in Minkowskian space and the Gowdy cosmological models, providing a rigorous definition of the propagator. Here, the impossibility of unitarily implementing some symplectic transformations turns out to be an obstacle to generalize the construction of semiclassical states through the eigenstates of the Lewis invariant [9]. Nevertheless, we have shown that the unitary implementability of the dynamics in appropriate Schrödinger representations allows us to define suitable semiclassical states for these systems. In the case of the Gowdy cosmologies, they can be used to probe the existence of large quantum gravity effects in several ways. For instance, one may construct suitable regularized operators to represent the (three- or four-dimensional) metric of these models by using arguments similar to those employed in the linearly polarized Einstein–Rosen waves [59–61] and the Schmidt model [13]. Calculating the expectation values of these operators in the coherent states, one may deduce the additional conditions (if any) that the sequences  $\mathbf{z} \in \ell^2(\mathbb{C})$  (see Theorem 6 in Section 5) should satisfy in order to admit an approximate classical behavior. It is also important to analyze if the metric quantum fluctuations are relevant for all states.

In addition, one may proceed as in [62] by appropriately promoting the quadratic invariant  ${}^{(4)}R_{abcd} {}^{(4)}R^{abcd}$  into a quantum mechanical operator. According to that reference, one should be able to unambiguously fix the operator order by requiring that the expectation values of this quantity in the coherent states exactly reproduce the classical results far from the singularities. In analogy with the results of [62], even if the expectation values in other states (such as linear combinations of coherent states) give nonclassical results, it is expected that the classical singularities persist in all cases. This physical consideration is supported by the purely quantum behavior of the uncertainties of the field and momentum operators in the coherent states at the classical spacetime singularities.

The most natural way to extend the analysis developed in this article consists in considering generic nonautonomous quadratic Hamiltonians which contain the time-dependent harmonic oscillators as particular cases. These systems can be analyzed from the perspective of some recent works on this subject (see [63–65]) in which Lie systems in quantum mechanics are studied from a geometrical point of view, developing methods to obtain the time evolution operators associated with time-dependent Schrödinger equations of Lie-type. These techniques may be successfully applied to infinite-dimensional quadratic Hamiltonian systems by following a functional description similar to the one performed in this article. In particular, the different resulting factorizations for the time evolution operators may be especially useful to define alternative families of semiclassical states for these systems.

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## Appendix A. Factorization of the evolution operator

In this appendix, we briefly summarize the construction of a well-defined factorization for the evolution operators of Minkowskian free fields and Gowdy cosmologies. The reader is referred to Section 5 to revise the notation and definitions. A particularly useful way to proceed is to factorize  $U(t, t_0)$  as [26]

$$U(t, t_0) = \mathcal{D}_\rho(t, t_0) \mathcal{R}_\rho(t, t_0) \mathcal{S}_\rho(t, t_0),$$

with

$$\mathcal{D}_\rho(t, t_0) := D_\rho^{-1}(t) D_\rho(t_0),$$

$$\mathcal{S}_\rho(t, t_0) := D_\rho^{-1}(t_0) S_\rho^{-1}(t) T_\rho(t_0),$$

$$\mathcal{R}_\rho(t, t_0) := T_\rho^{-1}(t_0) R_\rho(t, t_0) T_\rho(t_0),$$

where  $D_\rho(t)$  and  $S_\rho(t)$  are displacement and squeeze operators of the type defined in Section 3.2, in such a way that

$$\mathcal{D}_\rho^{-1}(t, t_0) a_\ell \mathcal{D}_\rho(t, t_0) = \left( 1 + i|\alpha_\ell|^2 \left( \frac{\dot{\rho}_\ell(t)}{\rho_\ell(t)} - \frac{\dot{\rho}_\ell(t_0)}{\rho_\ell(t_0)} \right) \right) a_\ell + i\bar{\alpha}_\ell^2 \left( \frac{\dot{\rho}_\ell(t)}{\rho_\ell(t)} - \frac{\dot{\rho}_\ell(t_0)}{\rho_\ell(t_0)} \right) a_\ell^*, \quad (73)$$

$$\begin{aligned} \mathcal{S}_\rho^{-1}(t, t_0) a_\ell \mathcal{S}_\rho(t, t_0) = & i \left( \beta_\ell \bar{\alpha}_\ell \frac{\rho_\ell(t_0)}{\rho_\ell(t)} - \alpha_\ell \bar{\beta}_\ell \frac{\rho_\ell(t)}{\rho_\ell(t_0)} + |\alpha_\ell|^2 \frac{\dot{\rho}_\ell(t_0)}{\rho_\ell(t_0)} \left( \frac{\rho_\ell(t)}{\rho_\ell(t_0)} - \frac{\rho_\ell(t_0)}{\rho_\ell(t)} \right) \right) a_\ell \\ & + i\bar{\alpha}_\ell \left( \bar{\alpha}_\ell \frac{\dot{\rho}_\ell(t_0)}{\rho_\ell(t_0)} - \bar{\beta}_\ell \right) \left( \frac{\rho_\ell(t)}{\rho_\ell(t_0)} - \frac{\rho_\ell(t_0)}{\rho_\ell(t)} \right) a_\ell^*, \end{aligned} \quad (74)$$

$$\begin{aligned} \mathcal{R}_\rho^{-1}(t, t_0) a_\ell \mathcal{R}_\rho(t, t_0) = & \left( \cos \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) + i \left( (\alpha_\ell \bar{\beta}_\ell + \beta_\ell \bar{\alpha}_\ell) \dot{\rho}_\ell(t_0) \rho_\ell(t_0) - |\alpha_\ell|^2 \left( \dot{\rho}_\ell^2(t_0) + \frac{1}{\rho_\ell^2(t_0)} \right) \right. \right. \\ & \left. \left. - |\beta_\ell|^2 \rho_\ell^2(t_0) \right) \sin \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) \right) a_\ell \\ & + i \left( 2\bar{\alpha}_\ell \bar{\beta}_\ell \dot{\rho}_\ell(t_0) \rho_\ell(t_0) - \bar{\beta}_\ell^2 \rho_\ell^2(t_0) - \bar{\alpha}_\ell^2 \left( \dot{\rho}_\ell^2(t_0) + \frac{1}{\rho_\ell^2(t_0)} \right) \right) \sin \left( \int_{t_0}^t \frac{d\tau}{\rho_\ell^2(\tau)} \right) a_\ell^*, \end{aligned} \quad (75)$$

and similarly for  $a_\ell^*$ . Here, the solutions  $\rho_\ell$  to the EP equations are conveniently selected as follows. For the Minkowskian free fields we choose  $\rho_\ell(t) = 1/\sqrt{|\ell|}$ ; for the 3-torus Gowdy model, we take

$$\rho_\ell(t) = \sqrt{\frac{\pi t}{2} \left( J_0^2(|\ell|t) + Y_0^2(|\ell|t) \right)}, \quad (76)$$

whereas for the 3-handle and the 3-sphere Gowdy models we choose

$$\rho_\ell(t) = \sqrt{\frac{\sin t}{2} \left( \pi \mathcal{P}_\ell^2(\cos t) + \frac{4}{\pi} \mathcal{Q}_\ell^2(\cos t) \right)}. \quad (77)$$

Solutions (76) and (77) have the asymptotic expansions

$$\rho_\ell(t) = 1/\sqrt{|\ell|} + O(|\ell|^{-3/2}), \quad \dot{\rho}_\ell(t) = C(t)/|\ell|^{5/2} + O(|\ell|^{-7/2}),$$

as  $|\ell| \rightarrow +\infty$ . Here,  $C(t)$  is a function of time which depends on the spatial topology and whose form we do not need to specify. It is then straightforward to check the unitary implementability of the transformations (73)–(75) in the Hilbert space by following the arguments employed in Section 5.2.

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